UNIT I

INTRODUCTION OF SPECTROMETRY

Properties of electromagnetic radiation- wave properties – components of optical instruments – Sources of radiation – wavelength selectors – sample containers – radiation transducers – Signal process and read outs – signal to noise ratio - sources of noise – Enhancement of signal to noise - types of optical instruments – Principle of Fourier Transform optical Measurements.

INTRODUCTION

Analysis:

Analysis refers to the detailed examination of the elements or structure of something. Chemical analysis uses instruments and methods used to separate, identify, and quantify matter. **Analytical chemistry** is the science of obtaining, processing, and communicating information about the composition and structure of matter.

Analysis of two kinds.

- Qualitative analysis
- Quantitative analysis

Qualitative analysis

Qualitative analysis deals with the identification of elements or functional groups present in a sample. In short, quantitative analysis answers "What is it?"

Example: inorganic salt analysis (identification of cations and anions), organic elemental analysis, organic functional group analysis.

Quantitative analysis

Quantitative analysis deals with the quantification of the substance. It tells you how much substance is present. In short, quantitative analysis answers "How much is it?"

Example: Volumetric analysis (titrations)

Methods of analysis

- Classical method
- Instrumental method

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Classical methods of analysis

Classical methods are the techniques which are the fundamentals of laboratory practices. These are the traditional method of chemical analysis which is still being used by scientists even now. Classical method is cheaper and easily available for schools and industries. It is sometimes called as "wet chemistry" where there are too many chemical reactions are used to identify certain compounds. The classical method consumes more time than the instrumental analysis. These methods are often labour intensive. The results are often accurate and precise.

Examples:

 Quantitative analysis performed by gravimetric and volumetric (titrimetric) methods

Instrumental Analysis

Instrumental methods are often called modern method of analysis. The reason is that these analytical techniques use modern equipments such as computers and other electronic equipments.

Instrumental method is expensive because the machines are highly specialized for a particular chemical analysis. Quantitative results are often more accurate and precise than the classical methods. Precision is dependent less on the operator and more on the instrument and sources of noise. Not all schools and colleges can afford those machines. Machines used are quite sophisticated that experts are needed to operate the machines to avoid system malfunctioning.

Examples:

Qualitative analysis using GC, HPLC, NMR spectroscopy etc.

Instrumental methods of Chemical Analysis (vs classical techniques)

Advantages

- less labour intensive
- easy to automate
- simultaneous multi component analysis
- fast analysis
- lower detection limits

Disadvantages

- higher expense
- harder to trouble shoot problems, more technical expertise

Spectroscopy

Spectroscopy is one of the most powerful tool used to derive information about atomic and molecular structure. **Spectroscopy is the study of the interaction between matter and electromagnetic radiation.** It involves the study of radiation emitted, absorbed, transmitted or scattered by the matter under study. It provides valuable information regarding chemical structure such as functional groups, unsaturation, bond strength, molecular structure such as molecular symmetry, bond distances, bond angles etc.

Spectrometry

The term **Spectrometry** is used for the quantitative measurement of the intensity of one or more wavelengths in the electromagnetic radiation. It is the method used for the study of certain spectrums. Ion-mobility spectrometry, mass spectrometry, etc are some examples of spectrometry. In these cases, a spectrum does not necessarily mean a plot of intensity versus frequency. For example, the spectrum for mass spectrometry is the plot between intensity (number of incident particles) versus the mass of the particle. Spectrometers are the instruments used in spectrometry. The operation of each type of instrument depends on the form of spectrometry used in the instrument.

What is the difference between Spectrometry and Spectroscopy?

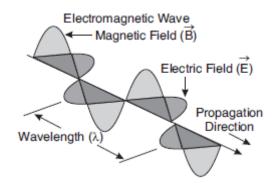
- Spectroscopy is the science of studying the interaction between matter
 and radiation while spectrometry is the method used to acquire a
 quantitative measurement of the spectrum (metry means measurement).
- Spectroscopy does not generate any results. It is the theoretical approach of science. Spectrometry is the practical application where the results are generated.

Electromagnetic radiation

Electromagnetic radiation (**EMR**) is a form of energy transmitted through space at very high velocities. This energy has wave nature and is associated with both

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electric and magnetic fields and hence, the name. Electric and magnetic field oscillate perpendicular to each other and both are perpendicular to the direction of propagation of wave.



Properties of electromagnetic waves

- Electromagnetic waves are composed of oscillating electric and magnetic fields at right angles to each other and both are perpendicular to the direction of the propagation of the wave.
- Do not require a medium for transmission.
- Travel at the speed of light (3 × 10⁸ ms⁻¹) in vacuum.
- Have no mass.
- Electromagnetic waves are transverse waves.
- Neither deflected by electric nor magnetic fields.
- Follow the laws of reflection and refraction.
- Energy of electromagnetic waves is directly proportional to its frequency.

Some important characteristics of wave

Every wave has five important characteristics, namely, wavelength (λ), frequency (ν), velocity (c), wave number (ν –) and amplitude (a).

- Wavelength (λ): The distance between two neighbouring troughs or crests is known as wavelength. It is denoted by λ and is commonly expressed in nanometers (1 nm = 10^{-9} m) or Angstrom (1 Å = 10^{-10} m).
- Frequency (v): The frequency of a wave is the number of times a wave passes through a given point in a medium per second. It is denoted by

vand is expressed in cycles per second (cps) or hertz (Hz) 1Hz = 1cps. The frequency of a wave is inversely proportional to its wavelength (λ).

$$v \propto 1/\lambda$$
 or $v = c/\lambda$

• **Velocity(c):** The distance travelled by the wave in one second is called its velocity. It is denoted by *c* and is expressed in ms⁻¹.

$$c = v\lambda$$
 or $\lambda = c/v$

Wavenumber (v): It is defined as number of wavelengths per cm. It is
denoted by v and is expressed in cm⁻¹.

$$\overline{v} = \frac{1}{\lambda}$$

• Amplitude(a): It is the height of a crest or depth of a trough of a wave and is denoted by a. It determines the intensity or brightness of the beam of light.

ELECTROMAGNETIC SPECTRUM

The **electromagnetic spectrum** is the distribution of electromagnetic radiation according to energy or wavelength.

The types of electromagnetic radiation are broadly classified as:

- 1. Gamma radiation 2. X-ray radiation 3. Ultraviolet radiation 4. Visible radiation
- 5. Infrared radiation 6. Microwave radiation 7. Radiowaves(According to decreasing energy or increasing wavelength)

Region	Wavelength (Angstroms)	Frequency (Hz)	Energy (eV)
Radio	> 109	< 3 × 10 ⁹	< 10 ⁻⁵
Microwave	$10^9 - 10^6$	$3 \times 10^9 - 3 \times 10^{12}$	$10^{-5} - 0.01$
Infrared	$10^6 - 7000$	$3 \times 10^{12} - 4.3 \times 10^{14}$	0.01 - 2
Visible	7000 - 4000	$4.3 \times 10^{14} - 7.5 \times 10^{14}$	2 – 3
Ultraviolet	4000 - 10	$7.5 \times 10^{14} - 3 \times 10^{17}$	$3-10^3$
X-Rays	10 - 0.1	$3 \times 10^{17} - 3 \times 10^{19}$	$10^3 - 10^5$
Gamma Rays	< 0.1	> 3 × 10 ¹⁹	> 10 ⁵

Some characteristics of different regions of the spectra

Types of EM waves	Source	Applications	
Radiowaves	Transmitter	Communication, transmitting radio and tv programmes.	
Microwaves	Microwave transmitter	Communication, cooking food.	
Infrared	Stars and other hot objects	Thermal imaging, night vision camera, remote control security system etc.	
Visible light	Stars, hot objects, flame	Normal vision, photography, photosynthesis.	
Ultraviolet	Stars, special lamps	Astronomical observations, killing microbes, security.	
X-rays	X-ray machine	Imaging, medical diagnosis, security system.	
Gamma rays	Radioactive decay	Sterilization, medical tracers, kill cancer cells.	

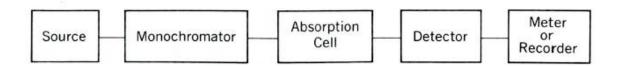
COMPONENTS OF OPTICAL INSTRUMENTS

Components of Optical Instruments Optical spectroscopic methods are based upon a) Absorption b) Scattering and c)Emission

Although the instruments for measuring each differ somewhat in configuration, most of their basic components are remarkably similar.

Components of typical spectroscopic instruments:

- 1. A stable radiation source
- 2. Wavelength selector
- 3. Sample container (cell)
- 4. A radiation detector
- 5. A signal processor and readout



1. RADIATION SOURCE

For proper measurements the radiation source must have following characteristics.

 It must generate a beam of sufficient power for ready detection and measurement.

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- Source should provide continuous radiation in the region being studied.
- Source should be stable over long periods of time.
- Source should emit measurable signal throughout the region.

Sources of visible radiation: The most common visible radiation source is incandescent tungsten filament lamp.

Sources of uv radiation: Hydrogen and deuterium lamps are most common sources used in uv spectroscopy. Deuterium lamp produces continuous radiation of higher intensity under same operating conditions when compared to hydrogen lamp.

Sources of infrared radiation: Nernst glower (a mixture of ZrO_2 , Y_2O_3 and Er_2O_3) and globar (SiC) are most widely used. Nichrome wire (near IR and IR) and Tungsten filament (near IR) can also be used

Source of electromagnetic radiation can also be classified according to whether they produce continuous or non continuous (line) spectra.

Continuous spectra: Continuum sources emit radiation that changes in intensity only slowly as a function of wavelength. Most of the sources are incandescent. Continuous sources are widely used in absorption and fluorescence spectroscopy.

Examples: Lamps of hydrogen, deuterium etc.

Line spectra: These are the sources that emit a discrete wavelength (few discrete lines) required for some instrumental applications. They are widely used in atomic absorption, atomic and molecular fluorescence, Raman, polarimetry and refractometry.

Examples: Na and Hg vapor lamps, Hollow cathode lamps, Electrode less discharge lamps, LASERS

LASERS: LASER is a source of monochromatic radiation available in visible and infrared region. Ruby laser, a simple and common type, has a rod-shaped cavity made of a mixture of solid aluminum oxide and chromium.

RUBY LASER

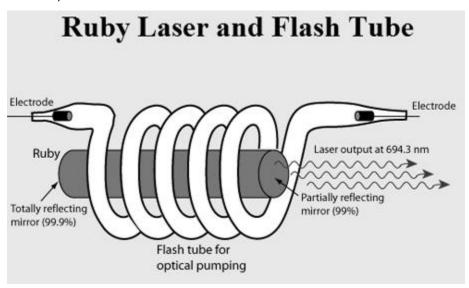
Ruby is a crystal of aluminium oxide (Al_2O_3) in which some of Al^{3+} ions are replaced by Cr^{3+} ions by doping. These Cr^{3+} ions give the crystal a pink or red

color depending upon the concentration of Cr^{3+} ions. Laser rods are prepared from a single crystal of pink ruby which contains 0.05% (by weight) chromium. Al_2O_3 does not participate in the laser action. It only acts as the host.

The ruby crystal is in the form of cylinder. Length of ruby crystal is usually 2 cm to 30 cm and diameter 0.5 cm to 2 cm. As very high temperature is produced during the operation of the laser, the rod is surrounded by liquid nitrogen to cool the apparatus.

Active medium or active center: Chromium ions act as active centers in ruby crystal. So it is the chromium ions that produce the laser.

A helical flash lamp filled with xenon is used as a pumping source. The ruby crystal is placed inside a xenon flash lamp. The flash tube fires and injects light into the ruby rod. The light excites atoms in the ruby. Thus, optical pumping is used to achieve population inversion (more number of species in excited state than in ground state) in ruby laser. A spontaneous emission photon by Cr^{3+} ion initiates the stimulated emission by other Cr^{3+} ions in metastable state producing a monochromatic intense beam of laser light. Thus various stages of laser production involves i) population inversion (optical pumping ii) spontaneous emission and iii) stimulated emission.



2. WAVELENGTH SELECTOR

Wavelength selectors are important instrumental components that are used to obtain a certain wavelength or a narrow band of wavelengths. It is so important in quantitative techniques as it ensures greater sensitivity (other regions does not interfere).

An ideal wavelength selector would output a single (line) wavelength or frequency of radiation. Realistically this is impossible. Wavelength selectors output a limited, narrow, continuous group of wavelengths called a **band**.

Two methods are commonly adopted for the selection of wavelength

- Filters
- Monochromators

a) FILTERS

Filters are wavelength selectors that usually allow the passage of some wavelengths but absorbs wholly or partially other wavelengths.

Properties of Filters

- 1. Simple, rugged (no moving parts in general)
- 2. Relatively inexpensive
- 3. Can select some broad range of wavelengths

Most often used in

- field instruments
- 2. simpler instruments
- 3. instruments dedicated to monitoring a single wavelength range.

It can be divided into two categories: Absorption filters, cutoff filters, interference filters and interference wedges.

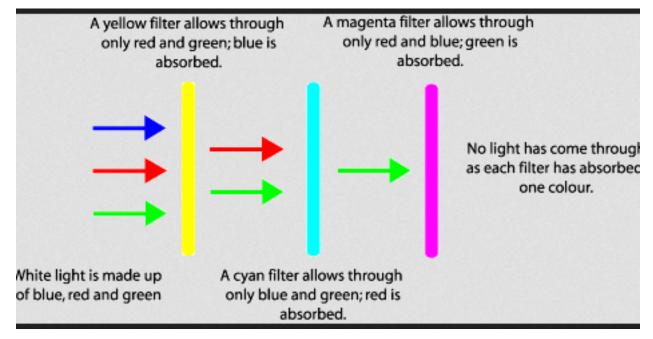
Absorption filters: This type of filters absorbs most incident wavelengths and transmits a band of wavelengths. Sometimes, they are called **transmission filters**.

Absorption filters are cheap and transmit a band of wavelengths with an effective bandwidth (the effective band width is the width of the band at half height) in the

range from 30-250 nm. Absorption filters are also combined and used to obtain a narrow range.

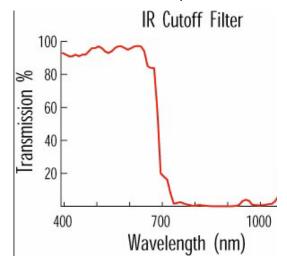
Their transmittance is usually low where only about 10-20% of incident beam is transmitted. Commonly used in visible spectrophotometry.

Example: colored glasses or plastics, dye suspended in gelatin. Sometimes, a combination of two colored filters are also used.



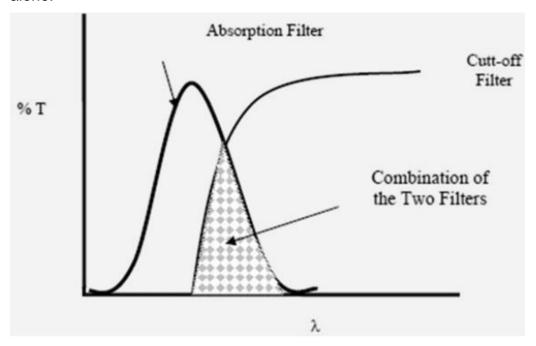
Cutoff filters:

With cut-off filters, the transmission of radiation is nearly 100%. However, this is only achieved for a specific band of wavelengths and transmission rapidly decreases to zero over the remainder of the spectrum.



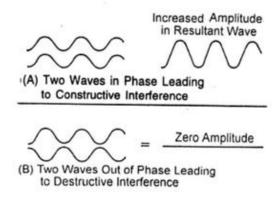
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Usually, cut-off filters are not used as wavelength selectors but are used in **combination with absorption filters** to decrease the bandwidth of the absorption filter. Only the common wavelengths of the two filters will be transmitted which will achieve a much narrower bandwidth than absorption filters alone.



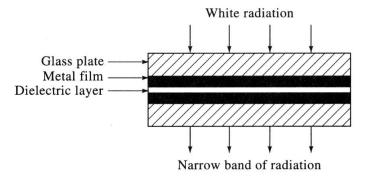
Interference filters:

Interference filters and wedges are based on the phenomenon interference. Interference is a phenomenon in which two waves superpose to form a resultant wave of greater, lower, or the same amplitude.



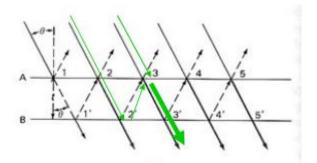
Interference filters (also called Fabry-Perot filters) rely on constructive and destructive interference in order to select a narrow bandwidth of radiation.

An interference filter is composed of a transparent dielectric, like calcium fluoride, sandwiched between two semitransparent metallic films. The array is further sandwiched between two glass plates to protect the filter. The thickness of the dielectric and the reflectivity of the metallic films are carefully selected because these factors control the transmitted wavelengths. Incident polychromatic radiation hits the filter at right angles and the transmitted beam will have a very narrow bandwidth. The structure of the interference filter can be depicted as in the figure below:



Working:

- Radiation hits filter → some reflected, some transmitted (transmitted light reflects off bottom surface)
- If proper radiation λ \rightarrow reflected light in phase with incoming radiation: other λ undergo destructive interference
- i.e., λ s of interest \rightarrow constructive interference (transmitted through filter); unwanted λ s \rightarrow destructive interference (blocked by filter)
- Result: narrow range of λ s transmitted



Schematic to show constructive interference

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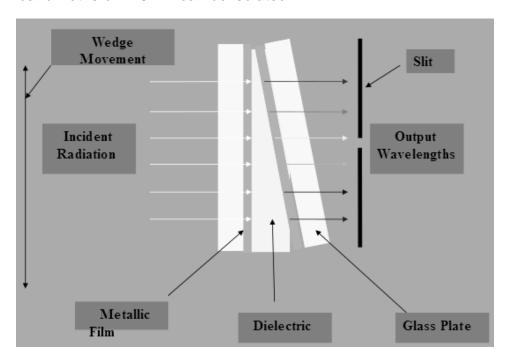
They are available for the visible region, the near-infrared region, and for several parts of the infrared region.

Advantages:

- Allow a much narrower band of wavelength to pass and are similar to monochromator in selectivity.
- Simpler and less expensive.
- Can be used with high intensity light sources.
- Continuous selection is possible by using wedge filter.

Interference wedge filter

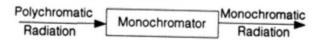
- Several interference filters are necessary to cover the entire visible range
 of the spectrum. This is not convenient as we would have to interchange
 filters according to wavelength of interest.
- To overcome this problem, a wedge machined dielectric was used. The
 dielectric in this case has different thicknesses and thus can transmit a
 wide range of wavelengths accordingly.
- A wedge dielectric of different thicknesses can transmit a wide range of wavelengths without having to change the interference filters in an instrument. By choosing the correct position on the wedge, variable bandwidths of ~20 nm can be isolated.



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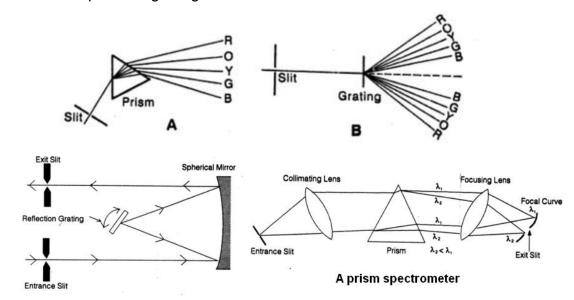
MONOCHROMATORS

Monochromator is used to separate a polychromatic radiation into suitable monochromatic form. Monochromator is a device that resolves a radiation into its component wavelengths and permits the isolation of any desired portion of the spectrum.



Monochromator has the following components

- Entrance slit: Slit is positioned on the way of radiation which deflects the beam and admits beam to pass through. It provides rectangular optical image.
- Collimating lens or mirror: It makes light beams parallel.
- Dispersing device (Prism or grating): Most widely used dispersive devices are prism or grating.



A simple grating monochromator

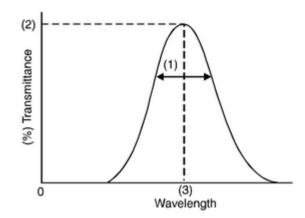
Virtually all modern instruments incorporate grating in their monochromators because gratings are cheaper and disperse radiation linearly as a function of wavelength.

• **Focusing device:** Again a lens or mirror is used for focusing the desired radiation towards the exit slit.

• Exit slit: Isolate the wavelength band of interest.

Three quantities determine the merit of monochromator

- Effective bandwidth: It is the width of the transmittance band at half of the transmission value.
- **Peak percent transmittance:** It shows percentage transmittance at the central wavelength.
- Central wavelength: It is the wavelength corresponding to the centre of the effective bandwidth.



PRISMS:

A prism is a wavelengths selector. Ability of prism to separate white light into its colour components is based on the wavelength dependence of the refractive index of the prism material.

Prisms refract light at the surface of two interfaces creating angular dispersion, and can be used to disperse ultraviolet, visible, and infrared radiation. Dispersion is the variation of refractive index with wavelength, or frequency. Since a beam of a polychromatic light is composed of several wavelengths, the dispersion of these wavelengths will be different when they are transmitted through the prism.

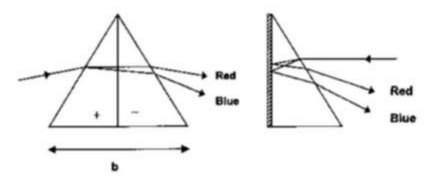
TYPES OF PRISM

Two common types of prisms can be identified:

a) Cornu Prism: It is a 60° prism which is made either from glass or quartz. When quartz is used, two 30° prisms (one should be left handed and the other is right handed) are cemented together in order to get the 60° prism. This is necessary since natural quartz is optically active and will rotate

light either to right or left hand. Cementing the left and right handed prisms will correct for light rotation and will transmit the beam in a straight direction.

b) Littrow Prism: A littrow prism is a 30° prism which uses the same face for input and dispersed radiation. The beam is reflected at the face perpendicular to base, due to presence of a fixed mirror. A littrow prism would be used when a few optical components are required.



The Cornu prism (left) is made of right and left handed quartz prisms in order to minimise the polarization effect. A Littrow prism (right) goes to form a half of the Cornu prism. Similar functioning is effected by silvering one side of the prism

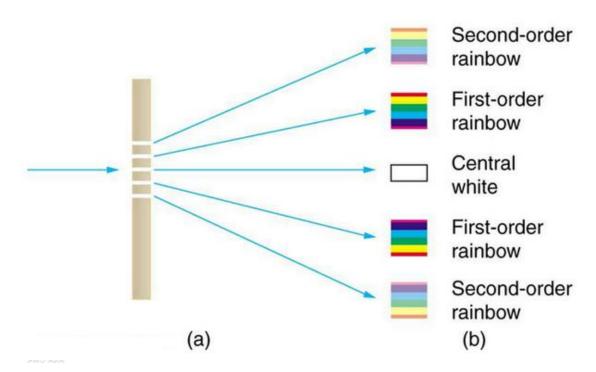
It should be always remembered that glass is nontransparent to uv radiation. - Therefore, when radiation in the ultraviolet is to be dispersed, a quartz prism, rather than a glass prism should be used. Quartz serves well in both UV and Visible.

GRATING:

Gratings have the same ability to separate light into its various wavelength components as prisms. However, gratings do not operate according to the principle of dispersion but works on interference and diffraction.

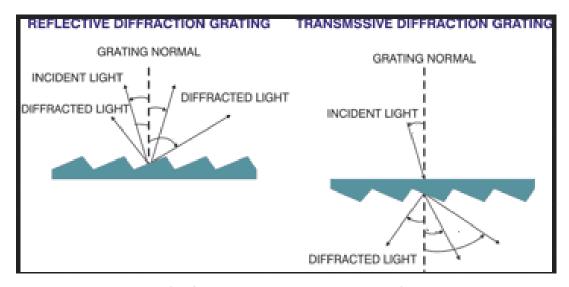
Grating is an optically flat polished surface that has dense parallel grooves. Parallel grooves are usually cut into a aluminum plate using a sharp point of a diamond or by laser. Line density may be as high as thousands of lines per millimeter.

Using a **diffraction grating** provides more slits, which increases the interference between the beams.



Two types of gratings are usually used:

- 1) transmission and 2) reflection (diffraction) gratings.
- Transmission grating: These are designed to disperse incident light at specific angles. A transmission grating is made of a transparent substance, so that the diffracted light goes through the grating and strikes a screen/detector/etc. on the other side. Angular dispersion is a function of angle of incidence and groove spacing. Dispersion increases as angle of incidence increases or as groove spacing decreases. They are seldom used in spectroscopic instruments.
- Diffraction or reflection grating: A reflection grating is made of a reflective/opaque substance; so the diffracted light bounces off and strikes a screen/detector/etc. on the same side. Almost all gratings, which are used in conventional spectroscopic instruments, are of the reflection type. The groove density can be as low as 80 to several thousand (6000) lines/mm.



Two common types of reflection gratings can be identified:

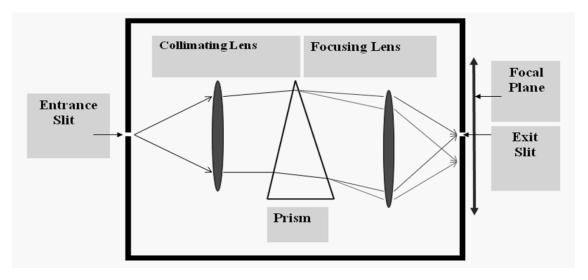
Echellette Gratings: Typical echellette gratings contain from 300 to 2000 lines/mm but an average line density of about 1200 to 1400 lines/mm is most common. The echellette grating uses the long face for dispersion of radiation. It is the grating of choice for molecular spectroscopic instruments.

Echelle Gratings: These have relatively coarse grooves (~80-300 lines/mm). They use the short face for dispersion of radiation and are characterized by very high dispersion ability. Echelle grating monochromators can produce highly pure spectral separations of radiation. Its light gathering power is about 25% times better than that of the echellette grating.

A monochromator is the part of instrument responsible for producing monochromatic radiation. Most essential component of any spectroscopic instrument and is composed of a prism or grating, as the selector, in addition to focusing elements; like mirrors or lenses. All these components are contained in a box that has an entrance and an exit slit. Two common types of monochromators can be described:

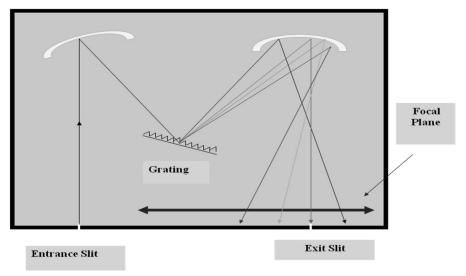
1. Bunsen Prism Monochromators (Prism based)

This type of monochromators uses a prism as the dispersion element in addition to two focusing lenses and two slits.



2. Czerney-Turner Grating Monochromator (Grating based)

This is composed of a grating, two concave mirrors and two slits. By moving the dispersing element or the exit slit, radiation of only a particular wavelength leaves the monochromator through the exit slit. By rotating the grating different wavelengths can be made to pass through the exit slit. The following setup can be associated with this monochromator system:



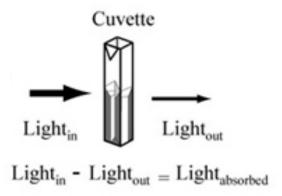
3. SAMPLE CELL

Sample cell or cuvettes that hold samples must satisfy three main requirements.

- The cells or cuvettes that hold the sample must be made of substances which are transparent in the special region of interest.
- It should not absorb much of the radiation.

 They must be reproducible in path lengths or their path lengths may be easily determined.

It is used for all spectroscopic studies except emission spectroscopy. Cuvettes come in many size and shapes but mostly cuvettes are 1cm x 1cm, so the light always goes through 1cm of the sample. Cells may be rectangular, cylindrical in shape.



Quartz or fused silica is used for making cells used in the ultraviolet region (below 250 nm). Silicate glasses can be employed in the region between 350 and 2000nm. Plastic containers are used in the visible region. Crystalline sodium chloride is the most common substance employed for cell windows in the infrared region.

Spectral Region	Material
UV	Fused silica
VIS	Plastic, glass
IR	NaCl

Sample cells should be cleaned thoroughly to prevent any contamination. Solution should be taken in adequate amount to avoid reflections from the upper surface. Presence of air bubbles should also be avoided.

4. RADIATION TRANSDUCERS (DETECTORS)

Transducers are devices which convert one form of energy to another. Usually they convert radiant energy (light intensity, temperature) into an electrical signal

(current or voltage) that can subsequently amplified, manipulated and finally converted into numbers proportional to the magnitude proportional to the original quantity.

There are no universal detectors that can be used for radiation of all frequencies. Three terms transducers, detectors and sensors are often used interchangeably. But there is a minor difference between these three.

Detector: This indicates change in environment (Smoke detector, Gas detector etc)

Transducer: It converts energy from one form to another, specifically from non electrical (light intensity, temperature etc) to electrical data. (Eg: Thermocouple converts temperature to voltage)

Sensor: It converts chemical data to electrical data (Eg:Biosensor converts biological activity into electrical data)

Characteristics of an ideal transducer are the following.

- Respond to radiant energy over a broad wavelength range.
- Sensitive to low levels of radiant power (high sensitivity).
- Electrical signal (S) produced is proportional to the radiant power (P)
- Electrical signal produced by it can be readily amplified.
- A high signal to noise ratio (S/N)
- A short response time (Fast response)
- Zero dark current: In absence of illumination, the detector output should read zero.
- Economic considerations

There are two general types of radiation transducers

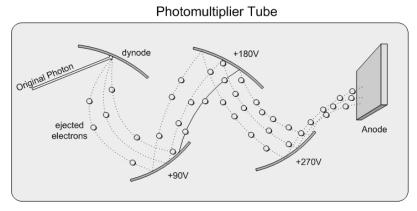
1. Photon detectors

2. Thermal detectors

1. Photon detectors

Photomultipliers, photovoltaic cells, phototubes etc are widely used photon detectors. They are faster and sensitive. Photoelectric detectors are commonly useful in ultraviolet, visible, and near infrared instruments.

a) Photomultipliers: Works on the principle of photon amplification. A photon strikes a photocathode using emission of electrons which are multiplied by striking a series of electrodes (dynodes). Dynode is covered by a material which emits several electrons (2-5) for each electron striking on its surface resulting in electron multiplication. A tube may have 9-16 dynodes. These secondary electrons produced are accelerated to the surface of another dynode which is maintained at a higher potential. The process is repeated several times. One photon of radiation results in 10⁶ to 10⁷ electrons reaching the anode. Thus, radiant energy is converted into electrical energy which can be easily measured.



Advantages:

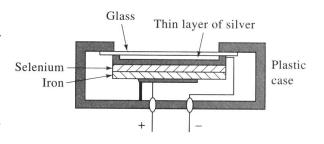
Fast response, very sensitive to low intensity.

Disadvantages:

Expensive, need high voltage power supply, sensitive to electromagnetic interference.

b) Photovoltaic (Barrier) cells: In this radiant energy gives a current at the interface of a semiconductor and a metal.

A semiconducting layer (Se) deposited on an iron or copper cathode and the semiconductor is coated with a thin metallic layer (Au or Ag), which serves as the anode. When radiation reaches the semiconductor, covalent bonds are broken resulting in conduction electrons



and holes. The electrons flow towards the metallic layer (anode) and the holes flow towards the base of the semiconductor (cathode). The electrons then flow

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through the circuit resulting in a current that is proportional to the power of the radiation. Maximum sensitivity at 550 nm and falls of at 350 nm and 750 nm, so they are most useful for visible radiation. It is cheap and is most commonly used in portable instruments.

Advantages:

Robust, cheap, rugged, good for portable instruments.

Disadvantages:

Not very sensitive, difficulty to amplify signal.

c) Phototubes: Phototubes are made of an evacuated glass or quartz envelope that has a semicylindrical cathode and a wire anode assembly. The cathode surface is coated with a layer of a photoemissive materials like Na/K/Cs. The voltage difference between the cathode and the anode is usually maintained at about 90 V. The incident beam hitting the cathode surface results in the emission of an electron and generates electric current proportional to radiation intensity. These electric current is amplified.

Phototube or photodiode

photocathode emitter (cathode) collector (anode)

photoelectrons

galvanometer measures current

Photons \rightarrow Electrons \rightarrow Current

Advantages:

This detector has better sensitivities than the barrier cell and does not show fatigue. The detector is good for the general detection of radiation intensity n the

UV-Vis region and is used in most low cost instruments. The transducer is also rugged and reliable.

2. Thermal detectors

It operates on the basis of heat detection. It is mainly used for infrared spectroscopy because photons in the IR region lack the energy to cause photoemission of electrons. Thermal detectors generally do not have as rapid a response as do photon detectors.

Three types of thermal detectors

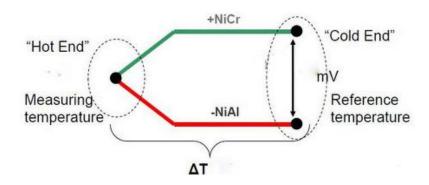
1. Thermocouples 2. Bolometers 3. Pyroelectric transducers

1. Thermocouples:

Thermocouple is a thermal detector made by two different metal wires joined at one end, this joint ends is placed in a temperature zone where temperature should be measured called "hot zone" and the other end of thermocouple where two metal wire are open(not connected or joined) placed in a low room temperature called "cold zone or reference temperature.".

Now two ends of this metal pair are placed in two different temperature zone. A net thermoelectric voltage is generated according to the temperature difference between two ends. This voltage is measured in the open pair placed in cold zone or reference zone.

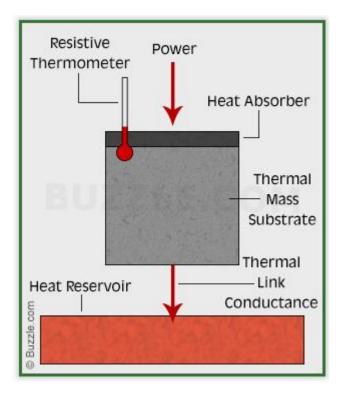
To enhance the performances of the thermocouples, often there are a number of thermocouples in series, perhaps as many as 100. The "hot" junctions are all attached close together. This type of device is called a **thermopile**.



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2. Bolometers: Constructed of strips of metal (platinum or nickel) whose resistance (Ω) changes as a function of temperature (resistance approximately increases 0.4% for every degree rise in temperature).

Working:



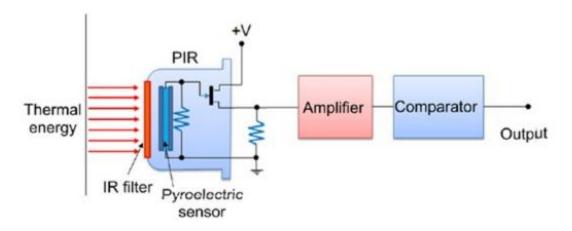
- A bolometer consists of an absorptive element, such as a thin layer of metal, connected to a thermal reservoir (a body of constant temperature) through a thermal link.
- Whenever radiation/heat hits the absorbent element, the power is absorbed, and the overall temperature of the element increases, heating up the thermal mass substrate.
- Through the connection between the substrate and the heat reservoir, the measure of the change in temperature is noted in the resistive thermometer. The calculation of the thermal input is equal to the ratio between the constant temperature of the heat reservoir and the variable temperature of the absorbent element.
- Used in thermal cameras to capture image, particle detectors, security devices etc.

Advantages:

- Can function effectively even at room temperature.
- In addition to photons and ionizing particles, they can also measure nonionizing particles.
- Compared to other particle detectors, these instruments are very sensitive, and give extremely accurate measurements of energy resolution.
- It gives a fast response, and can take sharp images of even moving objects.

3. Pyroelectric Transducers:

- Pyroelectricity is the ability of certain materials to generate a temporary voltage when they are heated or cooled. Constructed of crystalline wafers (triglycine sulfate, TGS) that have a strong, sensitive temperature dependent polarization.
- In presence of an electric field, when such a crystal material heats up, its electrical dipoles line up, called as polarization. On cooling, the material retains its polarization. In absence of electric field, when this polarized material is subjected to infra red radiation, its polarization reduces., which can be measured.



TGS crystals have fast response time and are commonly used in FTIR spectrometers.

5. SIGNAL PROCESS AND READ OUT

Signal processor: Signal processor modifies the signal into a form that is more convenient for the readout device. Signal may be filtered, amplified, converting from analog to digital, etc. This process is typically accomplished with amplifiers, ammeters, potentiometers and potentiometer recorders. Signal processors may also perform mathematical operations on signal such as differentiation, integration, conversion to logarithm, Fourier transform etc.

Techniques like photocounting are used when light incident on a photomultiplier tube becomes very low. Photon counting is used to detect very low-level-light such as Raman spectroscopy, fluorescence analysis, and chemical or biological luminescence analysis where the absolute magnitude of the light is extremely low.

Readout Device: Digital meters and computer monitors are some examples of read out devices. Computers are often used to control various instrumental parameters, to process and store data, to print results and spectra, to compare results with various database, and to communicate with other computers and network devices.

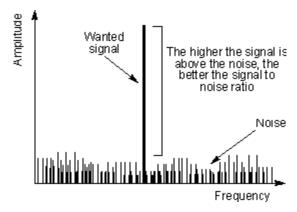
SIGNAL TO NOISE RATIO

Signal is what you are measuring that is the result of the presence of your analyte .**Noise** is extraneous information that can interfere with or alter the signal. It is the unwanted energy that interferes with the ability of the receiver to detect the wanted signal. Noise is considered as random. Noise free data can never be realized in the laboratory because some types of noise arise from thermodynamic and quantum effects that are impossible to avoid in any measurement.

Signal-to-noise ratio (SNR or S/N) is a measure that compares the level of a desired **signal** to the level of background **noise**. It is defined as the **ratio** of **signal** power to the **noise** power, often expressed in decibels.

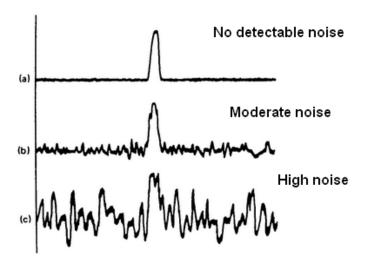
$$\mathrm{SNR} = \frac{P_{\mathrm{signal}}}{P_{\mathrm{noise}}},$$

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The electric signal should be directly related to the chemical or physical property being measured and that should be related to the amount of analyte present. So, ideally, when no analyte is present there should be no signal. In the absence of any noise, the baseline will be smooth.

Signal vs wavelength with different noise levels



For a DC signal like use mean value for signal and standard deviation of the noise:

$$\frac{\text{Signal}}{\text{Noise}} = \frac{\text{mean}}{\text{standard deviation}} = \frac{\overline{X}}{\overline{s}}$$

$$\frac{S}{N} = \frac{1}{RSD} \quad \text{RSD} = \text{Relative Standard deviation}$$

SNR is actually two level measurements, followed by a simple calculation. First, we measure the *output level* of the device under test with no *input signal*. Then

we apply a signal to the device and take another level measurement. Then we find the ratio.

$$S/N = \frac{Average signal amplitude}{Average noise amplitude}$$

In other words, S/N expresses the ability of an instrument to discriminate between signals and noise. Since many signals have a very wide dynamic range, S/N is often expressed in terms of logarithmic decibel scale. Due to the definition of decibel, the S/N gives the same result, independent of the type of signal which is evaluated (ie power, current, voltage).

A S/N ratio of 3 is usually the minimum that is acceptable. Amplification of signals does not improve the S/N ratio as noise also gets amplified.

Sources of noise in Instrumental Analysis

Every device has some amount of noise at its output. A small amount of noise may not objectionable if the output signal is very strong. In many cases, the noise may not be audible at all. But if the signal level is weak, even a very low noise level can have an adverse effect. Most experiments 'strength' noise (N) is constant and independent of signal (S) The % error in the signal become larger as signal get smaller. For this reason use the figure of merit Signal-to-noise (S/N) instead of just the noise to describe the performance of an instrument

Chemical Noise

From a source of uncontrollable variables in the chemistry like changes in pressure or temperature of reaction, light affecting photo reactions etc.

Instrumental Noise

These refer to the noise from instrumental components. These fall into following categories.

- 1. Thermal or Johnson Noise
- 2. Shot noise
- 3. Flicker or 1/f noise
- 4. Environmental noise

1. Thermal Noise or Johnson Noise

- Caused by thermal agitation of electrons and other charge carriers in any part of the electronics (resistors, capacitors, Integrated chips, transistors, wires, connections etc).
- Due to different velocities and movement of electrons in electrical components.
- Dependent upon both temperature and the range of frequencies (frequency bandwidths) being utilized.
- Can be reduced by reducing temperature (cooling) of electrical components. It can be fully eliminated at absolute zero.
- Narrowing bandwidth can decrease thermal noise but it will also slow the rate of the machine therefore increasing time required to make a reliable measurement.
- This noise is independent of frequency, also called "white noise" because present at all frequencies in a constant amount.
- Considered "white noise" occurs at all frequencies given by

$$v_{rms} = (4kTR\Delta f)^{1/2}$$
,

ν_{rms} is root-mean-square of noise voltage

∆f is Frequency bandwith

k is Boltzmann constant

R is resistance in Ohms of the resistive element

T is temperature in K

2. Shot noise

- Occurs when electrons or charged particles cross junctions (different materials, vacuums, etc.)
- Can be junctions between n and p material in a transistor, Electrons jumping across a vacuum in a vacuum tube, solder joints in the circuit board, etc.
- Arises because electrons are quanta of charge, and flow of charge across
 a junction is therefore a multiple quanta event, and has to be dealt with

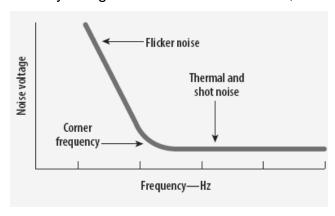
using statistics. Some of the electrons jump across the junction right away. Some of the electrons take their time jumping across the junction.

- This is also a white noise, uniform across all frequencies
- $i_{rms} = (2le \triangle f)^{1/2}$

So the i_{rms} noise in the current is due to I average direct current, E charge on the electron, Δf bandwidth of frequencies.

3. Flicker Noise

- This noise is frequency dependent, magnitude is inversely proportional to frequency. Hence also called 1/f noise.
- Easily recognizable as it depends on frequency.
- Significant at frequencies less than 100 Hz.
- Results in long-term drift in electronic components.
- Can be reduced by using resisters that are metallic, wire wound.



4. Environmental noise

- Compose of noise from surroundings.
- Sources are many.
- Can often be eliminated by identifying and eliminating the source
- Methods of eliminating it environmental noise include Moving the instrument elsewhere, controlling temperature in the room, eliminating interferences, turning off radios, TV's, other instruments etc.

Sources of noise and instruments

Typical Sources	Inexpensive photometers and spectrophotometers having small meters or digital displays	
Limited readout resolution		
Heat detector Johnson noise	IR and near-IR spectrophotometers and photometers	
Dark current and amplifier noise	Regions where source intensity and detector sensitivity are low	
Photon detector shot noise	High-quality UV-visible spectrophotometers	
Cell positioning uncertainties	High-quality UV-visible and IR spectrophotometers	
Source flicker	Inexpensive photometers and spectrophotometers	

Enhancement of signal to noise

To enhance the S/N ratio, either the noise must be reduced or the signal has to be enhanced or both should occur. Both Hardware and software methods can be used to improve S/N ratio.

When should you smooth a signal? There are two reasons to smooth a signal:

- (a) for cosmetic reasons, to prepare a nicer-looking or more dramatic graphic of a signal for visual inspection or publications, specifically in order to emphasize *long-term* behavior over *short-term*, or
- **(b)** when we have to measure the heights of peaks for analysis. Presence of high frequency noise may lead to not so accurate measurements.

Hardware methods: properly design instrument include choppers, shields modulators and other things in instrument design.

Software methods: computer algorithms to extract signal from under noise usually done with digital data so need to convert data from analog to digital, going to be done on a computer.

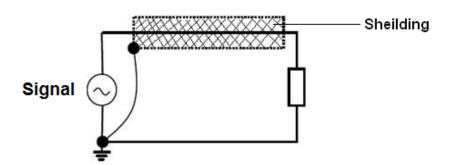
A. Hardware methods:

Hardware noise reduction can be done by incorporating into the instrument design components such as filters, choppers, shields, modulators, and synchronous detectors. These devices remove or attenuate the noise without affecting the analytical signal significantly. Hardware devices and techniques are as follows:

Types of Hardware:

a) Grounding and shielding:

Noise that arises from environmentally generated electromagnetic radiation can be substantially reduced by shielding, grounding and minimizing the length of conductors within the instrumental system. Shielding consists of surrounding a circuit, or some of the wires in a circuit with a conducting material that is attached to earth ground. Noise will be picked up by shield and not by circuit. Shielding is important when output of a high resistance transducer (glass electrode) is amplified.



b) Difference amplifiers:

Difference amplifiers can be used to attenuate (reduce) noise generated in the transducer. They selectively amplify the signal while reducing the noise in a transduced signal.

c) Analog filtering:

S/N ratio can be improved by the use of a low-pass analog filter.

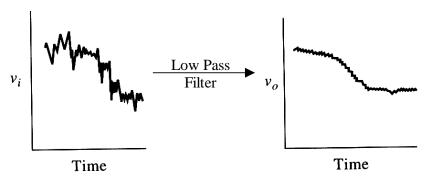
Types of analog filters:

- a. Low pass filters
- b. High pass filters
- c. Narrow band (band pass) filters

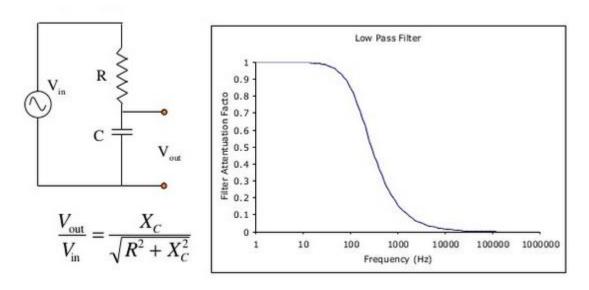
a. Low pass filters

Removes high frequency noise, such as shot and thermal noise, and allow low frequency signals to pass.

Useful with instruments that record low frequency analyte signals.



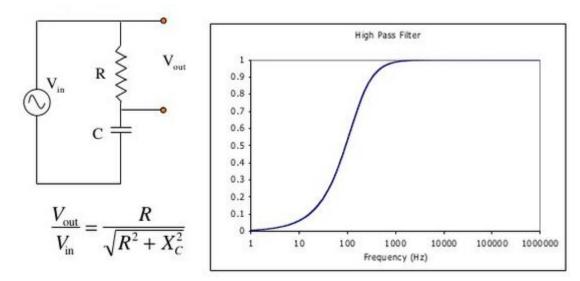
A series RC circuit functions as a low pass filter, when taking the output voltage across the capacitor. Here the ac signals at low frequency will pass unattenuated.



b. High pass filters

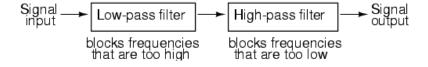
- Remove low frequency noise, such as flicker (1/f) noise and signal drift, and allow high frequency signals to pass.
- Useful with instruments that record high frequency analyte signals.

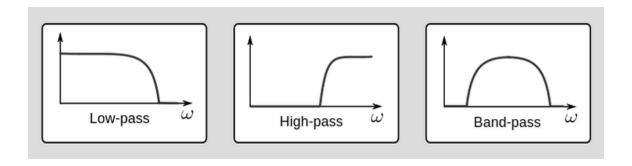
 A series RC circuit functions as a high pass filter, when taking the output voltage across the resistor. Here the ac signals at high frequency will pass unattenuated.



c. Narrow band (band pass) filters

- Remove all frequencies except for the frequency of interest. Or it allows only a certain frequency range to pass through.
- Filter circuits can be designed to accomplish this task by combining the
 properties of low-pass and high-pass into a single filter. The result is
 called a band-pass filter. In short, it's a combination of low pass and high
 pass filters.
- Creating a bandpass filter from a low-pass and high-pass filter can be illustrated using block diagrams:



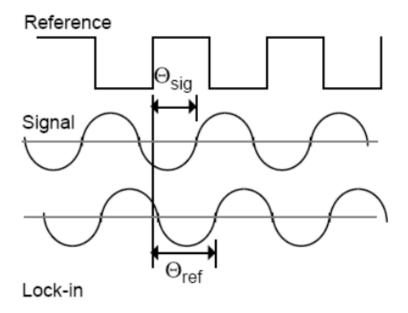


d) Modulation

Direct amplification of a low frequency or a dc signal is not easy when instrument exhibits flicker noise. So these signals are converted into higher frequency (modulation), then amplified and demodulated. Noise with frequency characteristic different from modulation-demodulation process is averaged to zero. Two commonly used methods are a) lock in amplifier and b) chopper amplifier.

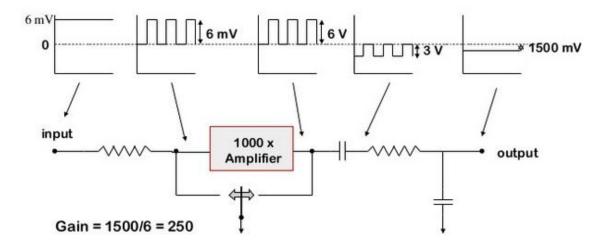
i) Lock in amplifiers

Lock-in amplifiers are used to detect and measure very small AC signals even up to a few nanovolts. Lock-in-amplifiers permit the recovery of signals even when the S/N is unity or less. It requires a reference signal that has the same frequency and phase as the signal to be amplified. A lock-in amplifier is generally relatively free of noise because only those signals that are locked-in to the reference signal are amplified. All other frequencies are rejected by the system.



ii) Chopper amplifier

An input dc signal is turned into a square wave similar to ac signal. It is then amplified and then demodulated and filtered to give amplified dc signal that avoids flicker noise. In this way, extremely small dc signals can be amplified.



B. Software:

Software methods are based upon various computer programs that permit extraction of signals from noisy data. Hardware convert the signal from analog to digital form which is then collected by computer equipped with a data acquisition module. These methods have become more common over the last 20 years with the advent of affordable high-speed microprocessors

and microcomputers. These methods have replaced or supplemented the hardware methods described in the previous section.

Three software methods most commonly used:

- 1. Ensemble averaging
- Boxcar averaging
- **3.** Digital filtering
 - a. Fourier transform
 - **b.** Least-squares polynomial smoothing

1. Ensemble Averaging:

Noise is randomly distributed, signal is not. So if we do a second experiment, signal will appear in same place but noise may not. So when we add up two runs signal increases but noise smoothens out. Signal increases by N but noise increases by \sqrt{N} . Hence S/N ratio increases by \sqrt{N} .

In ensemble averaging, successive sets of data stored in memory as arrays are collected and summed point by point. After the collection and summation are complete, the data are averaged by dividing the sum for each point by the number of scans performed. The signal-to-noise ratio is proportional to the square root of the number of data collected.

$$S_x = \frac{\sum_{i=1}^{n} S_i}{n}$$
 AND $N(\text{rms noise}) = \sqrt{\frac{\sum_{i=1}^{n} (S_x - S_i)^2}{n}}$

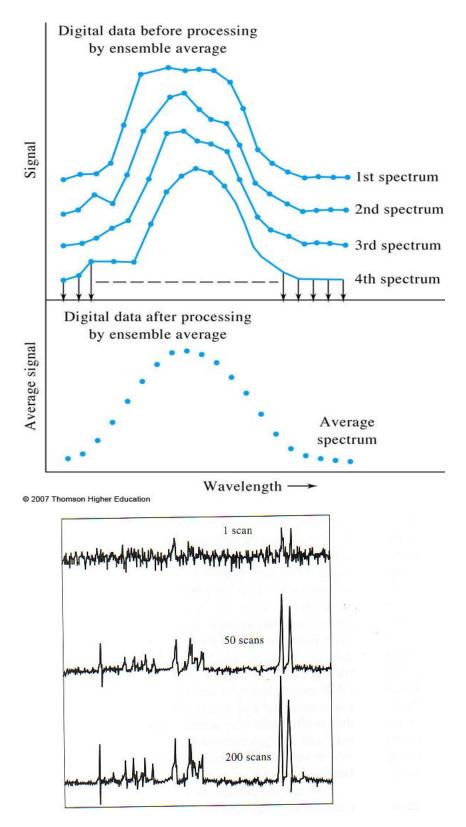
Where:

 S_x = average signal (point).

 S_i = individual measurement of the signal

n = number of measurements

$$\frac{S_x}{N} = \frac{S_x}{\sqrt{\sum_{i=1}^{n} (S_x - S_i)^2}} = \sqrt{n} \frac{S_x}{\sqrt{\sum_{i=1}^{n} (S_x - S_i)^2}}$$



2. Boxcar averaging

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Boxcar averaging is used for smoothing irregularities when signal varies slowly with time. It is assumed that the analog analytical signal varies only slowly with time and the average of a small number of adjacent points is a better measure of the signal than any of the individual points. In practice 2 to 50 points are averaged to generate a final point. This averaging is performed by a computer in real time, i.e., as the data is being collected. Its utility is limited for complex signals that change rapidly as a function of time.

As an example, consider a 3-point boxcar average of the following raw data:

First the data is divided into boxcars:

Then the averaging is performed:

$$(5 + 12 + 17) / 3 = 11.3$$

$$(18 + 21 + 22) / 3 = 20.3$$

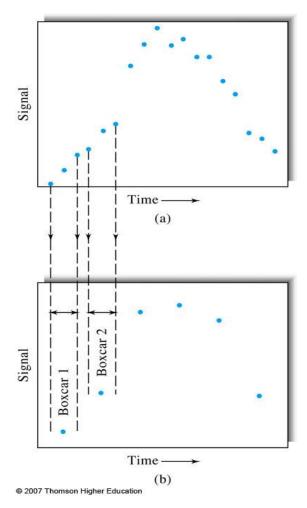
$$(25 + 30 + 35) / 3 = 30.0$$

$$(26 + 25 + 21) / 3 = 24.0$$

$$(15 + 13 + 8) / 3 = 12.0$$

This "smoothed" data can then be reported to the user:

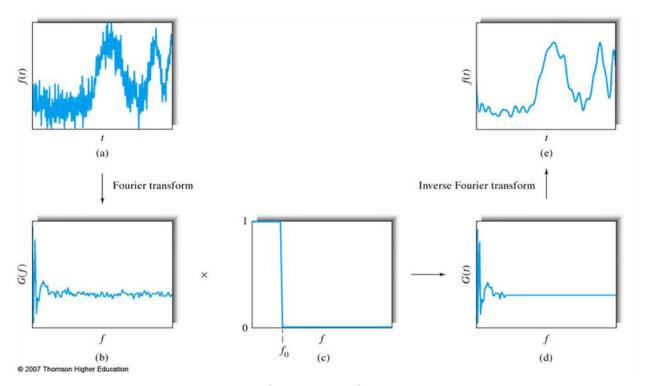
$$\{..., 11.3, ..., .., 20.3,, 30.0, ..., ..., 24.0, ..., ..., 12.0, ...\}$$



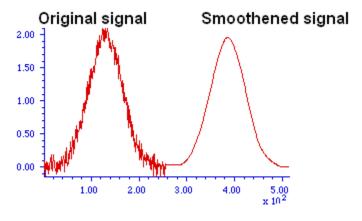
3. Digital filtering

Digital filtering can be accomplished by number of different well-characterized numerical procedure such as (a) Fourier transformation and (b) Least squares polynomial smoothing.

a. Fourier transform: Fourier transform is used to convert time domain data to frequency domain data, and vice versa. Here, in Fourier transform procedure the original signal which varies as a function of time (time domain signal) is converted to a frequency domain signal where the independent variable is frequency not time, accomplished mathematically on a computer by a Fourier transform. The frequency domain signal is then multiplied by the frequency response of a digital low pass filter which removes frequency components. The inverse Fourier transform then recovers the filtered time domain spectrum.



b. Least-squares polynomial smoothing: Least-squares polynomial smoothing is used to reduce high frequency noise in a low frequency wave form. This is very similar to the boxcar averaging but polynomial fitting is preformed repetitively over sections of the wave. In this process first 5 data points are averaged and plotted. Then moved one point to the right and averaged. This process is repeated until all of the points except the last two are averaged to produce a new set of data points. The new curve should be somewhat less noisy than the original data. The signal-to-noise ratio of the data may be enhanced by increasing the width of the smoothing function or by smoothing the data multiple times.



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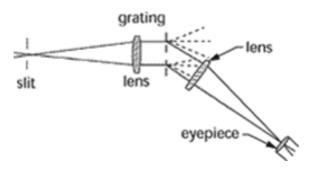
The noise is greatly reduced while the peak itself is hardly changed. Smoothing increases the signal-to-noise ratio and allows the signal characteristics (peak position, height, width, area, etc.) to be measured more accurately by visual inspection.

TYPES OF OPTICAL INSTRUMENTS

Different optical instruments comes with different nomenclatures. Most of the optical instruments have commons components like source, monochromator, detector etc mentioned earlier. Common nomenclatures are given below.

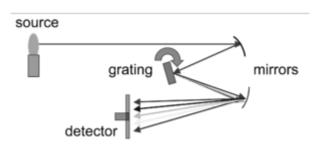
Spectroscope:

- An optical instrument used for the visual identification of atomic emission lines. Because atoms can absorb or emit radiation only at certain specific wavelengths defined by electron transitions, the spectrum of each type of atom is directly related to its structure.
- In its simplest form, a spectroscope is a viewing instrument consisting
 of a slit, a collimator, a dispersing element, and a focusing
 objective.
- Slit: Entrance of the beam
- Collimator: A collimator is a special type of lens that "straightens out" light coming in at various angles so that all of the light is travelling the same direction. The wavefront is converted into a planar wavefront.
- Dispersive element: Usually prism or grating
- Focusing objective: The focusing objective is just a lens system, such as that on a telescope, that magnifies the spectrum and focuses it for viewing by eye



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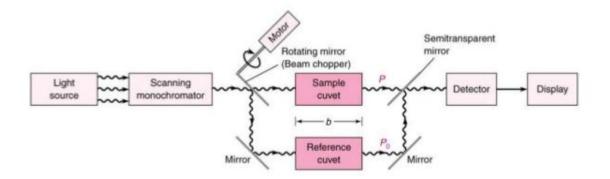
- A spectroscope gives useful information, but it is only temporary. To capture spectroscopic data permanently, the spectrograph was developed.
- Spectrograph: A spectrograph operates on the same principles as a spectroscope, but it contains some means to permanently capture an image of the spectrum. Early spectrographs contained photographic cameras that captured the images on film that is continuously exposed to the entire spectrum of dispersed radiation. Now photographic plates are replaced by diode arrays using a camera or charge coupled device (CCD) cameras that convert an optical signal into an electrical signal. They capture the image and transfer it to video or computer for further analysis.
- **Spectrometer:** A spectrometer is any instrument used to probe a property of light as a function of its portion of the electromagnetic spectrum, typically its wavelength, frequency, or energy.



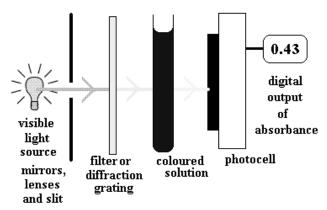
Spectroscope	Seeing	The first instruments for observing spectra were
		visual, and they were properly called
		spectroscopes.
Spectrograph Drawin	Drawing	When spectra began to be recorded on
	(recording)	photographic emulsions, just over a century ago,
		the instruments were called spectrographs . They
		did not measure - they produced an image, and
		other instruments (e.g., densitometers) took

		measurements from those images by measuring
		the photographic density (blackening) at points in
		the image.
Spectrometer	Measuring	When direct electronic measurements came in to
		replace the two-step process(recording and
		measuring), the instruments were called
		spectrometers.

Spectrophotometer: Spectrometer with a phototransducer (which converts light energy to electric energy) is called **Spectrophotometer**. It read relative intensities in the spectrum, rather than the wavelengths of emission/absorption. With most spectrophotometers, measurements can be done in both ultraviolet and visible region of the spectrum, which is not possible with colorimeters.



- Spectrofluorometer or spectrofluorimeter: It is a spectrophotometer for fluorescence analysis.
- Colorimeter: Instruments used for absorption measurement using one or more color comparison standards.



A simplified diagram of a colorimeter

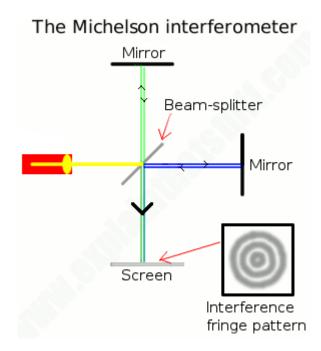
Photometer: A photometer is an instrument that measures intensity of Photometers measure absorption, scattering, photons. fluorescence, phosphorescence etc. Photometer consists of a source, filter, transducer, signal processor and read out. Photometer contains a filter instead of dispersive device. Wavelengths can only be changed by changing the filter. Some scientists refer photometers as colorimeters or **Photometers** photoelectric colorimeters. used for fluorescence measurements are also called fluorometers.

PRINCIPLE OF FOURIER TRANSFORM OPTICAL MEASUREMENT

Fourier transform is a techinique widely used in modern instruments. It is used in

- X-ray diffraction
- Electron microscopy (and diffraction)
- NMR spectroscopy
- IR spectroscopy
- Fluorescence spectroscopy
- Image processing
- Fourier transform is a mathematical technique that can be used to transform a function from one real variable to another (usually time domain to frequency domain).
- It is a unique powerful tool for spectroscopists because a variety of spectroscopic studies are dealing with electromagnetic waves covering a wide range of frequency.

- Being a transformation no image is created or lost in the process, so original image can be recovered by Fourier Transform and vice versa.
- Most machines uses "interferometer" for Fourier Transform. An
 interferometer is an instrument which uses the technique of
 superimposing (interfering) two or more waves to detect the differences
 between them. Michealson interferometer is widely used in FT-IR
 instruments.
- The interferometer produces a unique type of signal which has all of the infrared frequencies "encoded" into it. The signal can be measured very quickly, usually on the order of one second or so. Thus, the time element per sample is reduced to a matter of a few seconds rather than several minutes.



BASIC MATHEMATICAL TREATMENT

MR signal to be decomposed into a sum of sine waves of different frequencies, phases, and amplitudes. Fourier showed that any periodic signal s(t) can be written as a sum sine waves with various amplitudies, frequencies and phases.

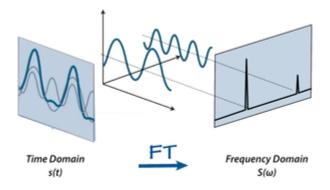
$$s(t) = a_0 + a_1 \sin(\omega t + \phi_1) + a_2 \sin(2\omega t + \phi_2) + a_3 \sin(3\omega t + \phi_3) + \cdots$$

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where $\mathbf{a_i}$'s are amplitudes, ϕ_i 's are phase shifts, and $\boldsymbol{\omega}$ is the **fundamental frequency**. The higher order frequencies 2ω , 3ω , etc. are called **harmonics**. For example, the Fourier expansion of a **square wave** can be written as

$$s(t) = \sin(\omega t) + \frac{1}{3}\sin(3\omega t) + \frac{1}{5}\sin(5\omega t) + \frac{1}{7}\sin(7\omega t) + \cdots$$

To realize this idea, Fourier transform from time domain to frequency domain is the essential process that enable us to translate raw data to readable spectra.

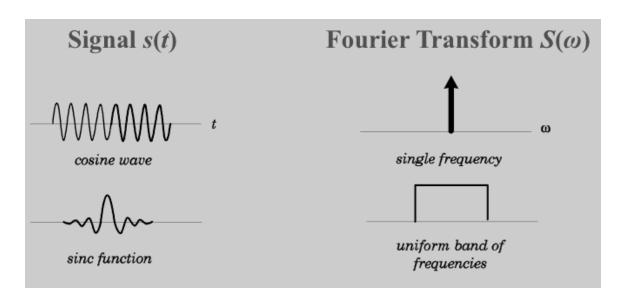


The *time domain* signal of the square wave, s(t), is shown on the left. The so-called *frequency domain* representation, $S(\omega)$, is shown on the right. $S(\omega)$ is called the *Fourier transform* of s(t). In general $S(\omega)$ is a complex-valued function composed of harmonic frequencies, phases, and their amplitudes obtained from the Fourier expansion.

Thus, Fourier transformation is the mathematical procedure connecting s(t) and $S(\omega)$. If s(t) is specified, $S(\omega)$ may be computed, and vice versa.

$$S(\omega) = \int_{-\infty}^{\infty} s(t)e^{-i\omega t}dt \qquad s(t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} S(\omega)e^{i\omega t}d\omega$$

The equation on the left is the Fourier Transform. That on the right is the *inverse* Fourier Transform.



Note that when s(t) is spread out in time, $S(\omega)$ is compact, and vice-versa.

Advantages of Fourier transform:

- Any space or time varying data can be transformed into a different domain called the frequency domain. This makes processing easier.
- Any function can be expressed as a sum of series of sine and cosines.
 Hence, you can easily study the function.
- Better Signal to noise ratio.
- Precise measurement.