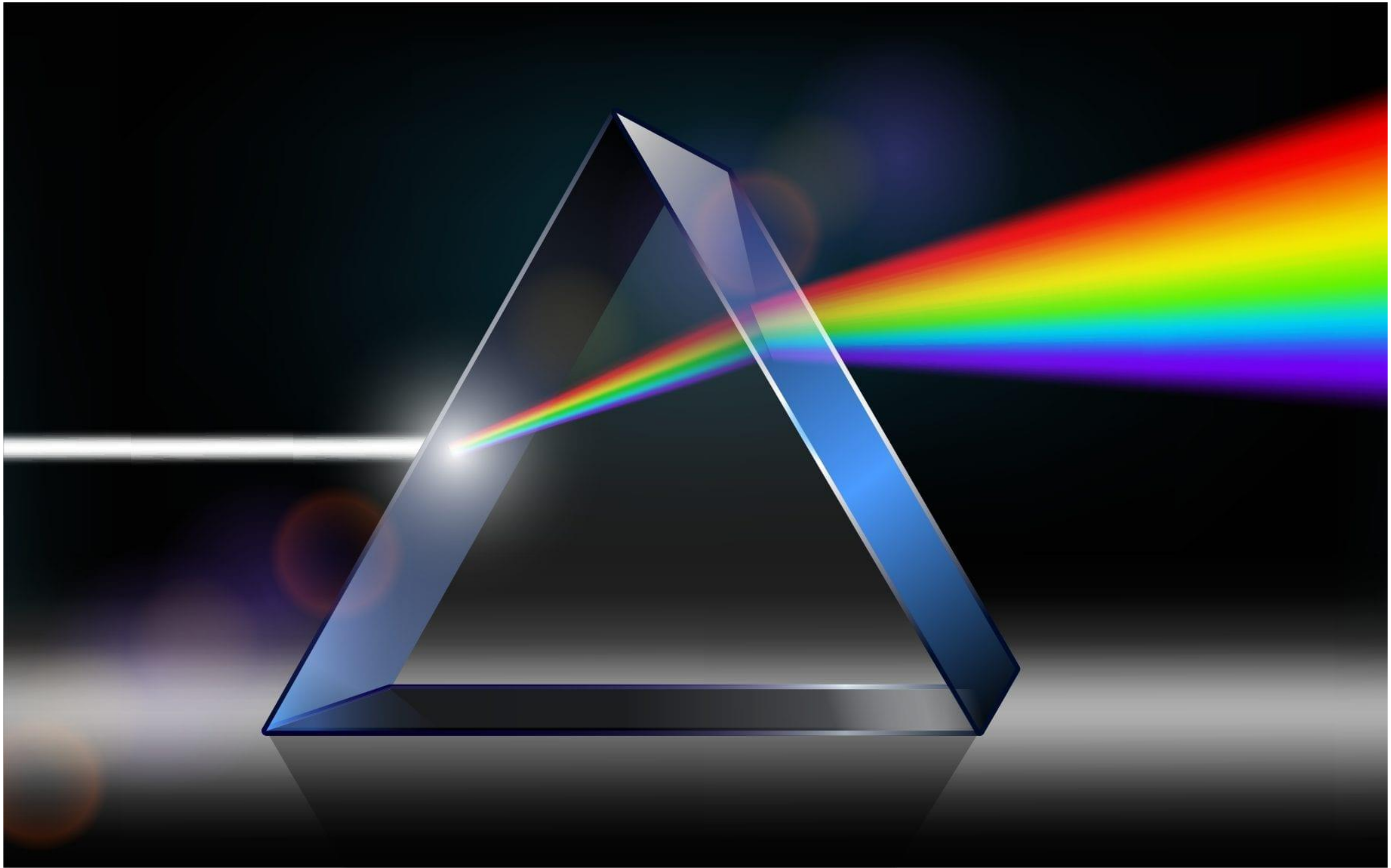
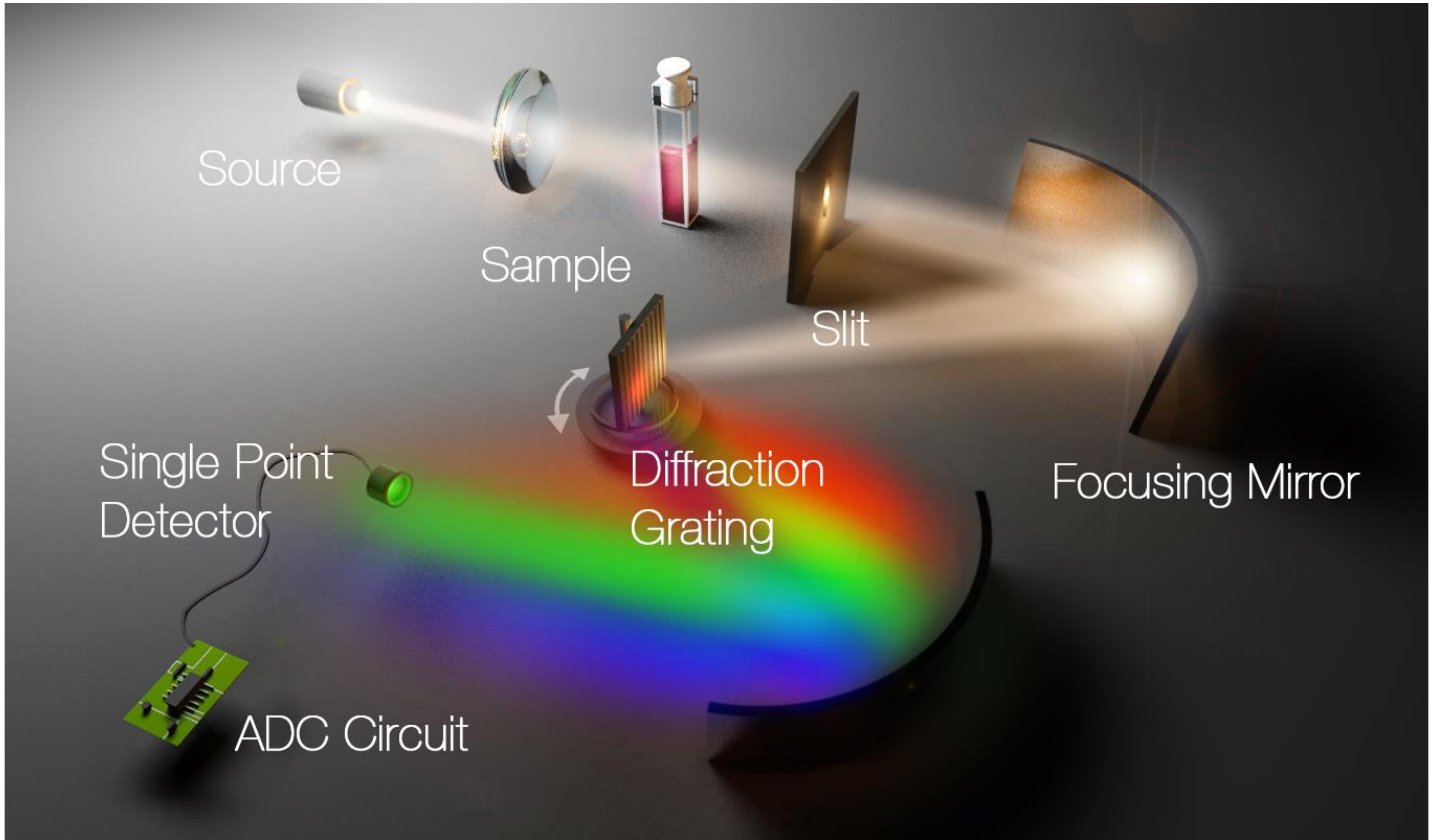
Spectroscopy



Spectroscopy

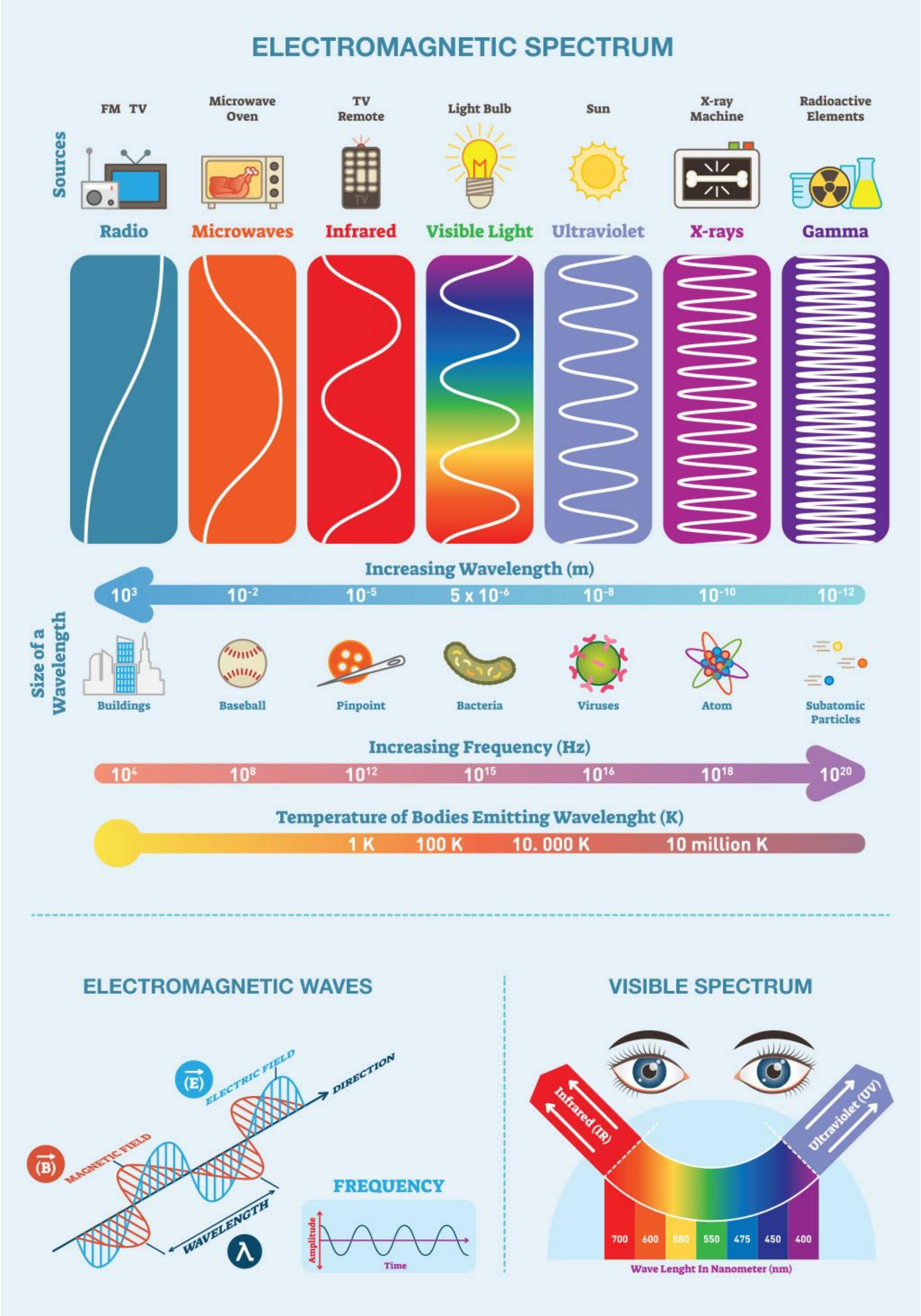
What is spectroscopy?

Spectroscopy is the scientific study of the **interaction between radiation (electromagnetic radiation, or light) and matter,** specifically how light is absorbed or emitted by different materials. It is used to identify and analyze the chemical composition, structure, and properties of substances by examining the patterns of wavelengths and frequencies of light that are emitted, absorbed, or scattered when the substance interacts with light. Spectroscopy also includes techniques that measure other properties of light, such as intensity, polarization, and phase, which provide important information about the physical and chemical processes occurring in materials.



Electromagnetic spectrum

The electromagnetic spectrum is a **range of all the types of electromagnetic radiation**. It is vast, covering everything from **radio waves, microwaves, infrared radiation, visible light, ultraviolet radiation, and X-rays, to gamma rays**. The electromagnetic spectrum is measured in wavelengths, which range from the long waves of radio waves to the short waves of gamma rays. **Each type of electromagnetic wave has a specific wavelength and frequency**, which determine how it travels and how it interacts with matter. The electromagnetic spectrum is used extensively in scientific research, medical imaging, and communication technologies.



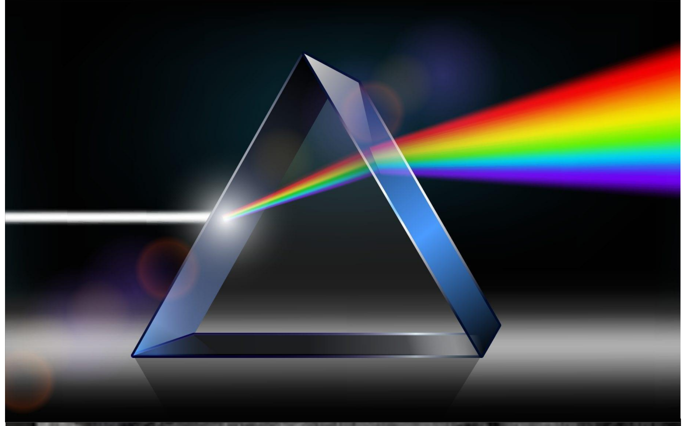
Spectroscopy: History

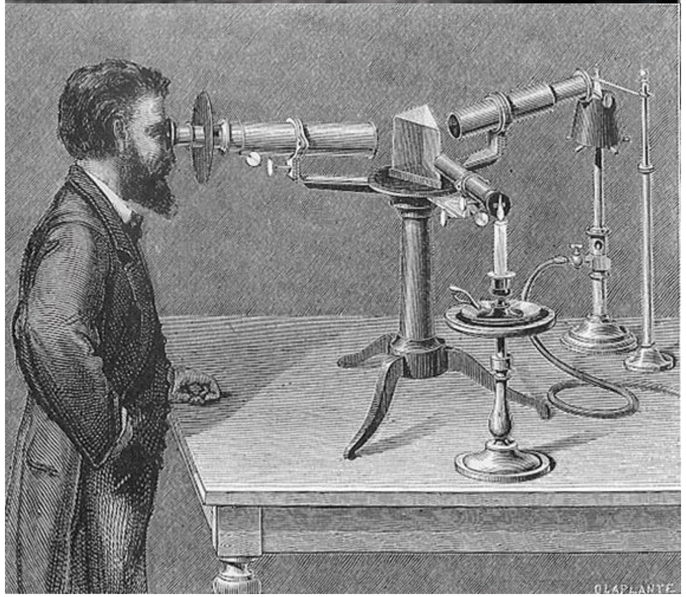
The origin of spectroscopy can be traced back to the 17th century when the Dutch physicist, Christian Huygens, discovered the phenomenon of diffraction. This led to the development of the prism and the realization that white light could be separated into its constituent colors.

In the early 1800s, the German physicist Joseph von Fraunhofer made significant contributions to the field of spectroscopy by studying the absorption of light by various substances. He discovered that the absorption lines in the spectrum of sunlight could be used to identify the chemical composition of materials.

In the mid-1800s, the German physicist Gustav Kirchhoff and his colleague Robert Bunsen developed the technique of spectroscopy using a spectroscope. They used this technique to identify the elements present in the sun by analyzing the spectrum of sunlight.

Over time, spectroscopy has become an essential tool in various fields, including chemistry, physics, biology, astronomy, and medicine. It has helped scientists gain a better understanding of the nature of matter and the universe.





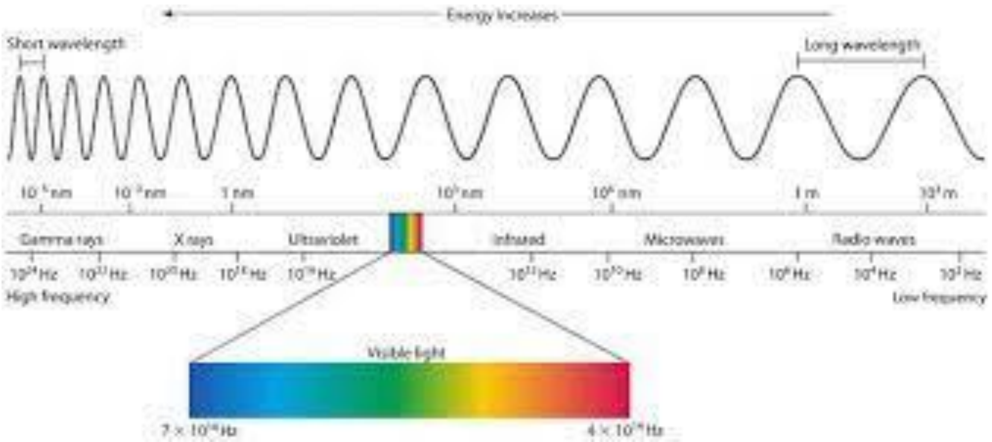
Classification of spectroscopy.

1. Type of radiative energy involved.

Spectroscopy can be classified in different ways based on the type of radiative energy, the nature of the interaction, or the measurement technique. They may **OVERLAP (a single technique be classified differently depending on the classification approach).**

One way to classify spectroscopy is by the **type of radiative energy involved**. This can range from gamma rays to radio waves in the electromagnetic spectrum. Some examples of spectroscopy based on this classification are:

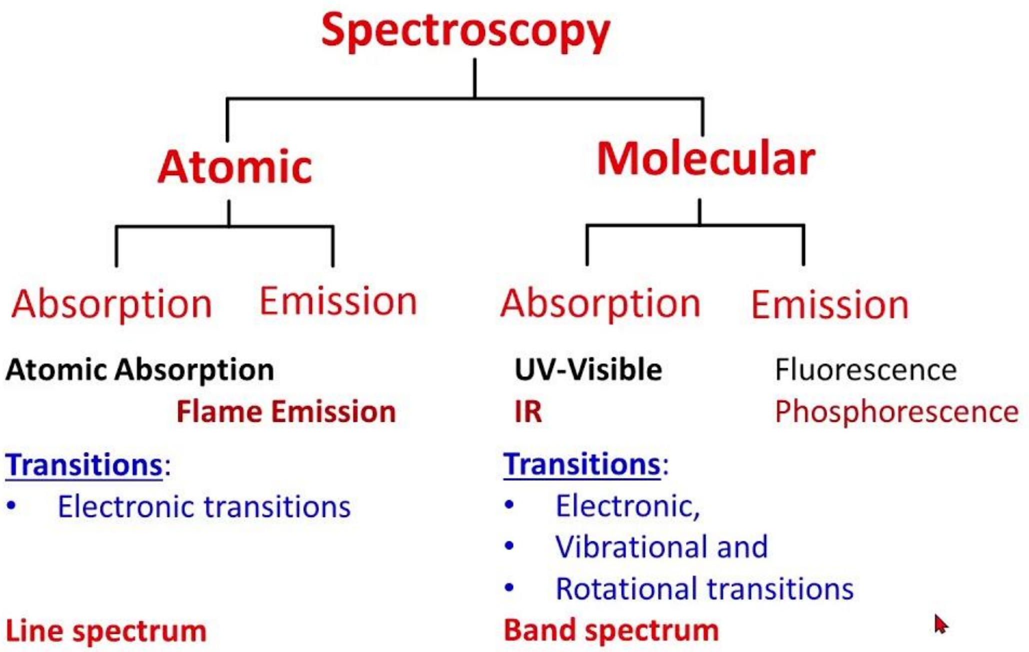
- **Gamma ray spectroscopy:** studies the gamma rays emitted by radioactive nuclei
- **X-ray spectroscopy:** studies the X-rays emitted or absorbed by atoms or molecules
- **Ultraviolet-visible spectroscopy:** studies the ultraviolet and visible light emitted or absorbed by atoms or molecules
- **Infrared spectroscopy:** studies the infrared radiation emitted or absorbed by molecules
- **Microwave spectroscopy:** studies the microwave radiation emitted or absorbed by molecules
- **Radiofrequency spectroscopy:** studies the radiofrequency radiation emitted or absorbed by nuclei or molecules

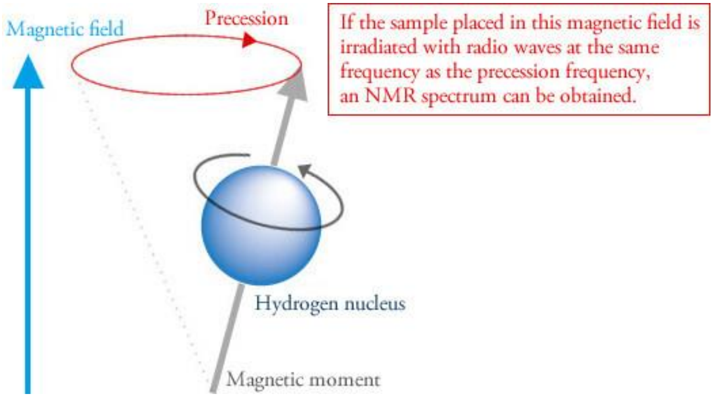


Classification of spectroscopy. 2. Type of interaction

Another way to classify spectroscopy is by **the nature of the interaction between matter and radiation**. This can involve different types of transitions, such as electronic, vibrational, rotational, nuclear, or molecular. Some examples of spectroscopy based on this classification are:

- **Atomic spectroscopy:** studies the electronic transitions in atoms
- **Molecular spectroscopy:** studies the vibrational and rotational transitions in molecules
- **Nuclear magnetic resonance (NMR) spectroscopy:** studies the nuclear spin transitions in magnetic fields
- **Electron paramagnetic resonance (EPR) spectroscopy:** studies the electron spin transitions in magnetic fields
- ~~**Mass spectrometry:**~~ studies the fragmentation of molecules by **ionizing radiation**



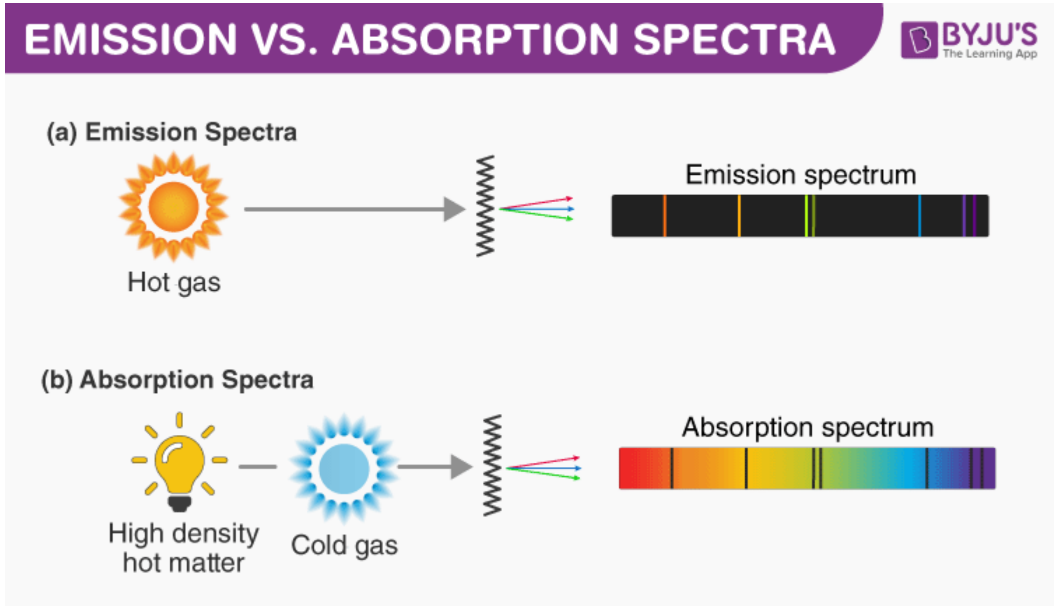


Classification of spectroscopy.

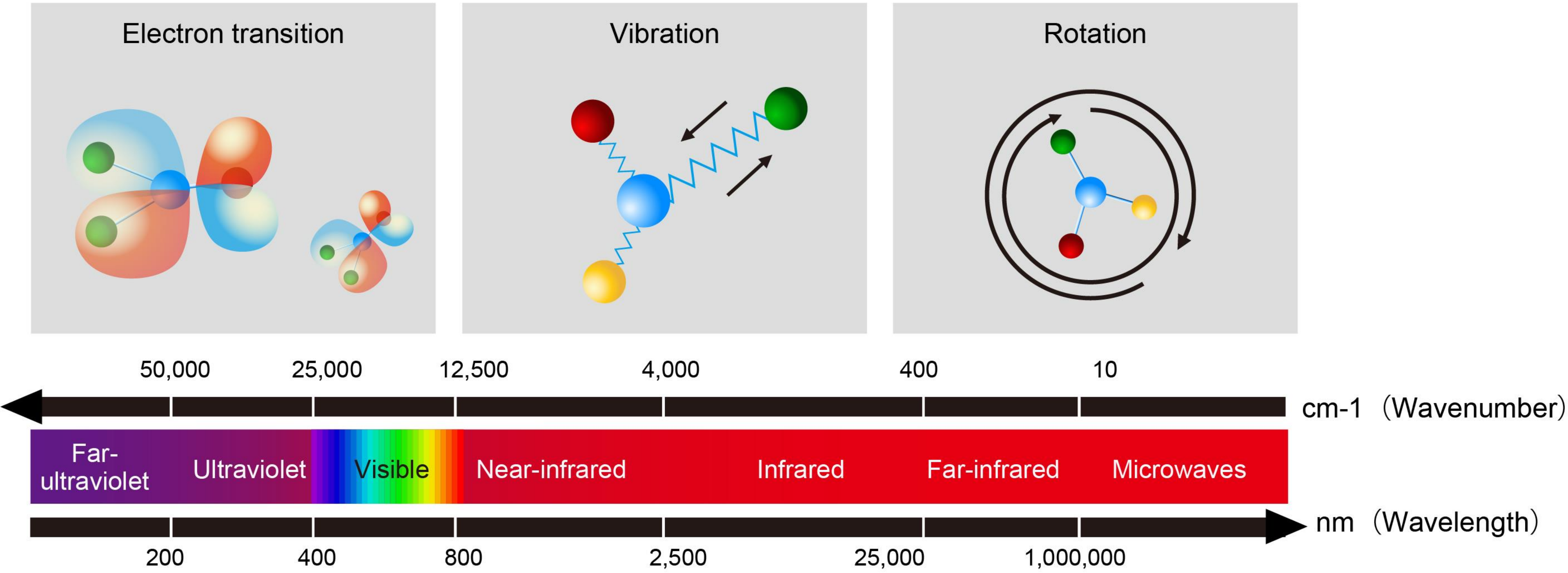
3. Type measurement technique.

A third way to classify spectroscopy is by the **measurement technique used**. This can involve different types of instruments, detectors, or methods of analysis. Some examples of spectroscopy based on this classification are:

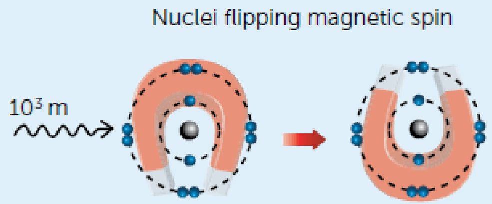
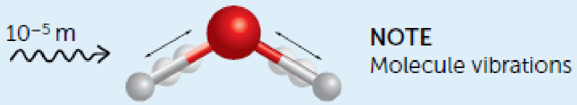
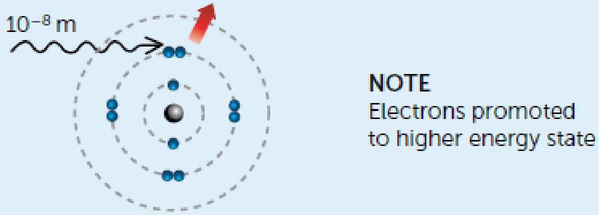
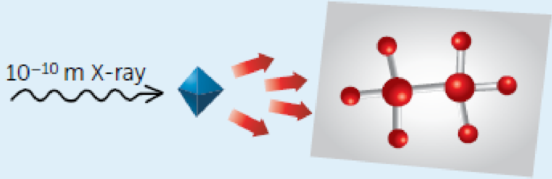
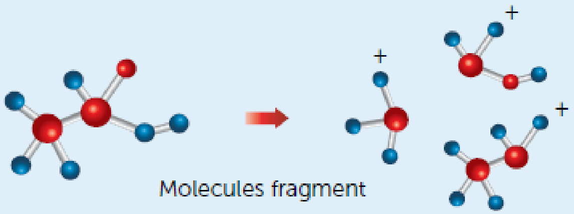
- **Emission spectroscopy:** measures the radiation emitted by a sample
- **Absorption spectroscopy**: measures the radiation absorbed by a sample
- **Reflection spectroscopy:** measures the radiation reflected by a sample
- **Scattering spectroscopy:** measures the radiation scattered by a sample
- **Fluorescence spectroscopy:** measures the radiation emitted by a sample after excitation by another radiation source
- **Fourier transform spectroscopy:** uses an interferometer to measure the interference pattern of radiation from a sample



Types of spectroscopy: Radiative energy involved



Types of spectroscopy

TECHNIQUE	RADIATION		WHAT CAN IT SEE?
Nuclear magnetic resonance (NMR) spectroscopy	Radio waves (10^3 m)		How neighbouring atoms of certain nuclei (e.g. 1H, 13C, 19F, 31P) in a molecule are connected together, as well as how many atoms of these types are present in different locations in the molecule.
Infrared spectroscopy	Infrared (10^{-5} m)		The functional groups that are present in a molecule.
Ultraviolet–visible spectroscopy	Ultraviolet (10^{-8} m)		Conjugated systems (i.e. alternating single and double bonds) in organic molecules as well as the metal–ligand interactions in transition metal complexes.
X-ray crystallography	X-rays (10^{-10} m)		How all the atoms in a molecule are connected in a three-dimensional arrangement.
Mass spectrometry	Non-spectroscopic technique		The mass to charge ratio of the molecular ion (i.e. the molecular weight) and the fragmentation pattern, which may be related to the structure of the molecular ion.

Atomic spectroscopy

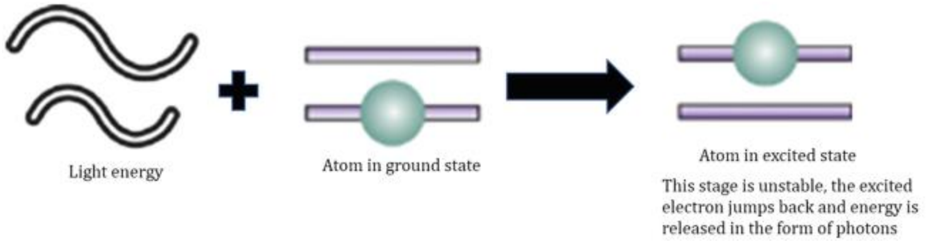
Atomic spectroscopy is a branch of spectroscopy that is used to analyze the **energy levels and spectra of atoms**. It is a technique that uses light and other forms of electromagnetic radiation to measure the interaction between light and material at an atomic level. It involves the absorption, emission, or scattering of electromagnetic radiation by the atoms of an element, and the resulting spectra can be used to identify the presence and concentration of specific elements in a sample.

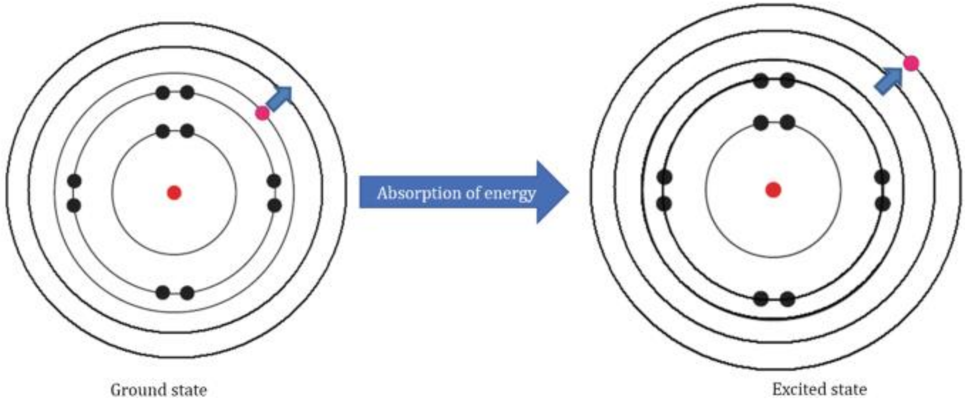
There are several types of atomic spectroscopy, including:

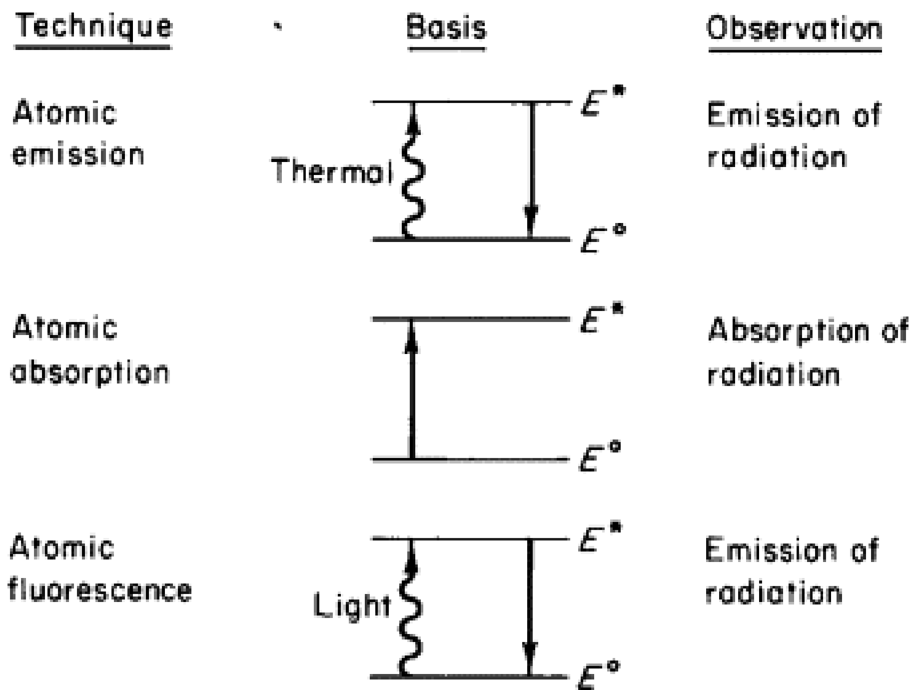
1. **Atomic absorption spectroscopy (AAS):** Measures the absorption of light by atomic vapors to identify and quantify the atoms present in a sample.

2. **Atomic emission spectroscopy (AES):** Measures the emission of light by atoms that have been excited by an external energy source, such as a flame or plasma.

3. **Atomic fluorescence spectroscopy (AFS):** Similar to AES but measures the fluorescence of atoms excited by an external energy source.







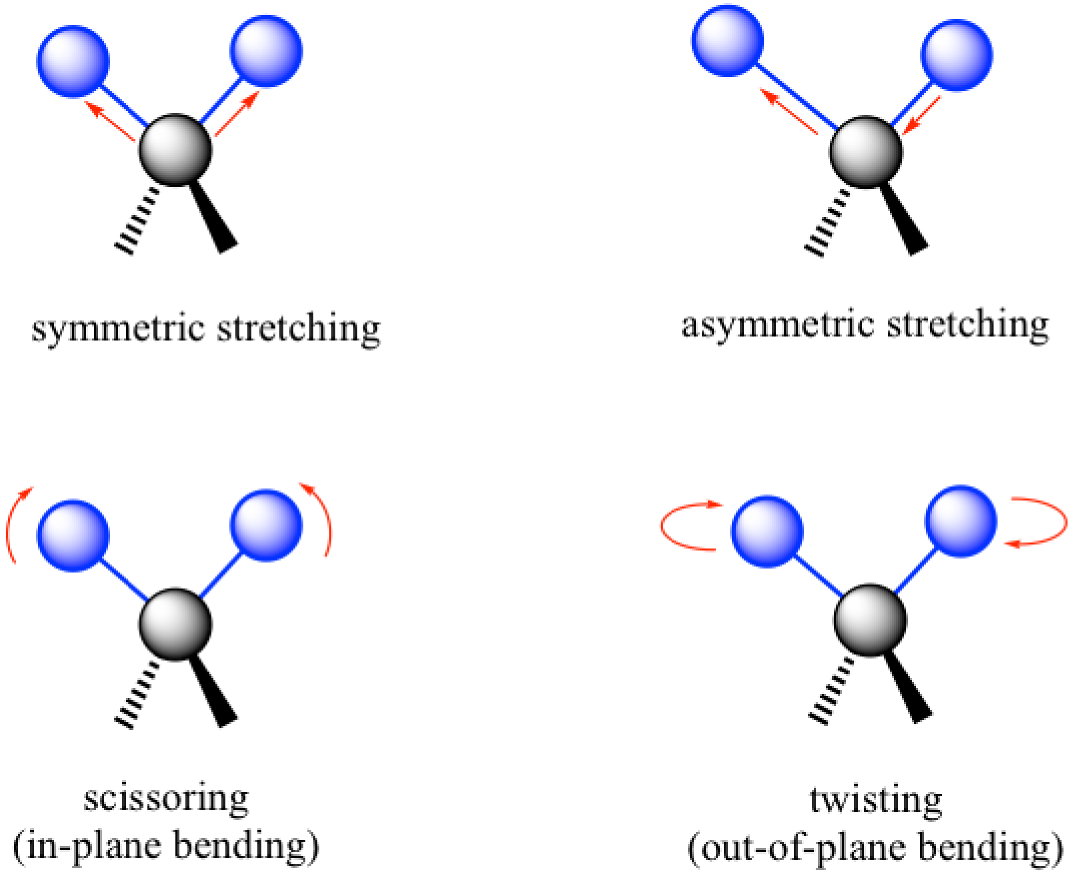
Molecular spectroscopy. I

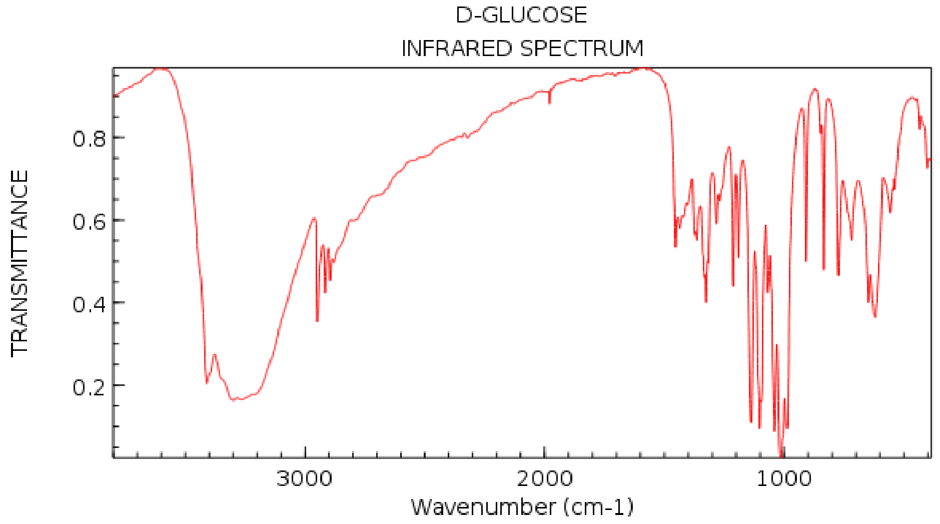
Molecular spectroscopy is a branch of spectroscopy that is used to study the interactions of molecules with electromagnetic radiation. It involves the use of light and other forms of electromagnetic radiation to measure the absorption, emission, or scattering of radiation by molecules. Molecular spectroscopy provides a way to identify and study the structure, properties, and behavior of molecules.

There are several types of molecular spectroscopy, including:

1. **Infrared spectroscopy**: Measures the absorption of infrared radiation by molecules to identify functional groups and compounds.

2. **Raman spectroscopy**: Measures the scattering of radiation by molecules to provide information about molecular vibrations and structure.





NIST Chemistry WebBook (http://webbook.nist.gov/chemistry)

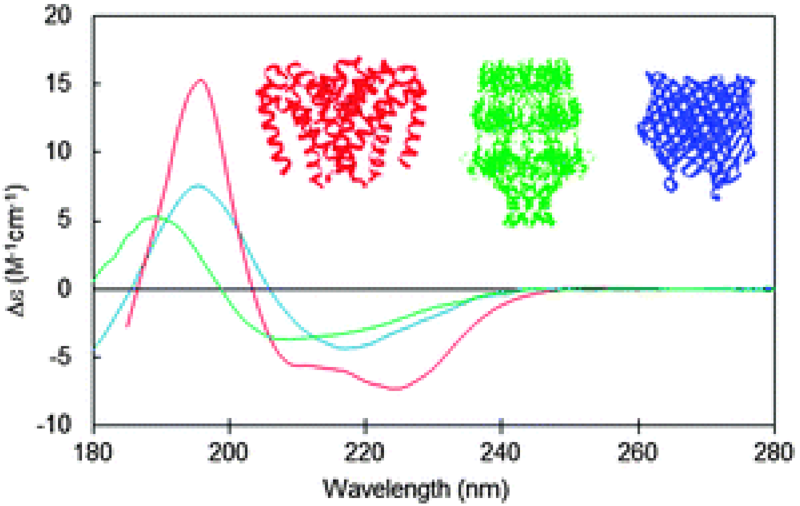
Molecular spectroscopy. II

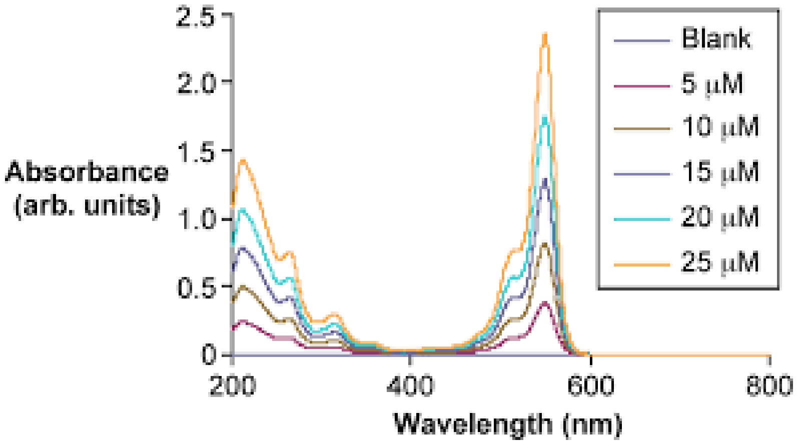
3. **UV-Visible spectroscopy:** Measures the absorption of ultraviolet and visible light by molecules to study electronic transitions and identify chromophores.

4. **Fluorescence spectroscopy**: Measures the fluorescence emitted by molecules after they have been excited by radiation to study molecular structure and dynamics.

5. **Circular dichroism spectroscopy:** Measures the difference in the absorption of left- and right-circularly polarized light by chiral molecules to determine their stereochemistry and conformation.

Molecular spectroscopy is widely used in various fields, including chemistry, biochemistry, materials science, and pharmacology, among others. It helps to identify and quantify molecules in complex mixtures, study molecular interactions, and determine the structure and dynamics of molecules in different environments.

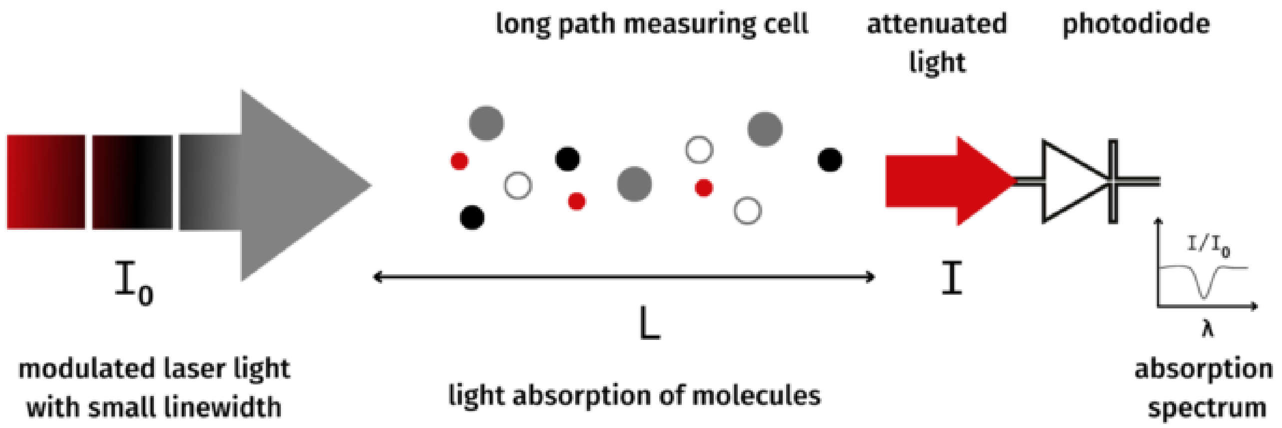




Absorption spectroscopy

Absorption spectroscopy is a technique that involves measuring the absorption of electromagnetic radiation by a substance over a range of wavelengths. This technique is widely used to identify the chemical composition and concentration of a sample. Absorption spectroscopy involves the **measurement of the intensity of light before and after it passes through a sample.** The difference in intensity is used to determine the amount of light absorbed by the sample, which in turn provides information about the concentration and properties of the sample.

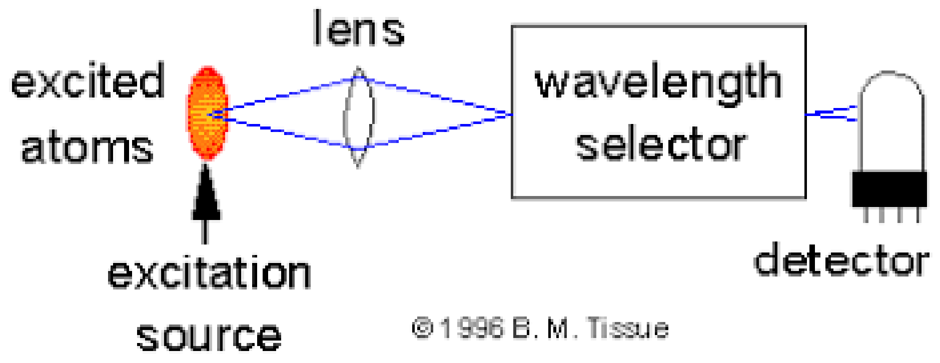
Absorption spectroscopy can be applied to the analysis of different types of samples, including liquids, gases, and solids. It can also be applied to the analysis of different types of molecules, including both organic and inorganic compounds. Examples of commonly used absorption spectroscopy techniques include infrared spectroscopy, UV-visible spectroscopy, and atomic absorption spectroscopy.



Emission spectroscopy

Emission spectroscopy is a technique that involves the **measurement of the electromagnetic radiation emitted by a substance.** This technique is used to identify the chemical composition and properties of a sample by analyzing the wavelengths of the emitted radiation. Emission spectroscopy involves the measurement of the intensity of light emitted by the sample over a range of wavelengths, which is then used to identify the types of atoms and molecules present in the sample.
Types:

1. **Atomic emission spectroscopy (AES):** This technique involves the analysis of the light emitted by excited atoms in a sample.
2. **Molecular emission spectroscopy**: This technique is used to analyze the light emitted by excited molecules in a sample (fluorescence, phosphorescence, chemiluminescence, etc.).
3. **Laser-induced breakdown spectroscopy (LIBS):** This technique involves the use of a laser to vaporize a small portion of a sample, which then emits light that is analyzed for elemental composition.
4. **Inductively coupled plasma emission spectroscopy (ICP-OES):** This technique involves the use of an inductively coupled plasma to excite atoms in a sample, which then emit light that is analyzed for elemental composition.
5. **X-ray fluorescence (XRF) spectroscopy**: This technique involves the use of X-rays to excite atoms in a sample, which then emit characteristic X-rays that are analyzed for elemental composition.



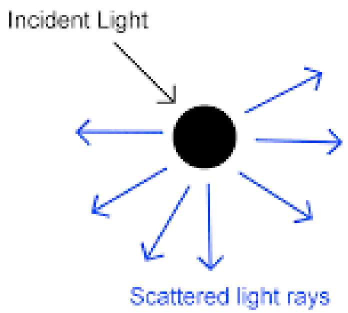
Scattering spectroscopy

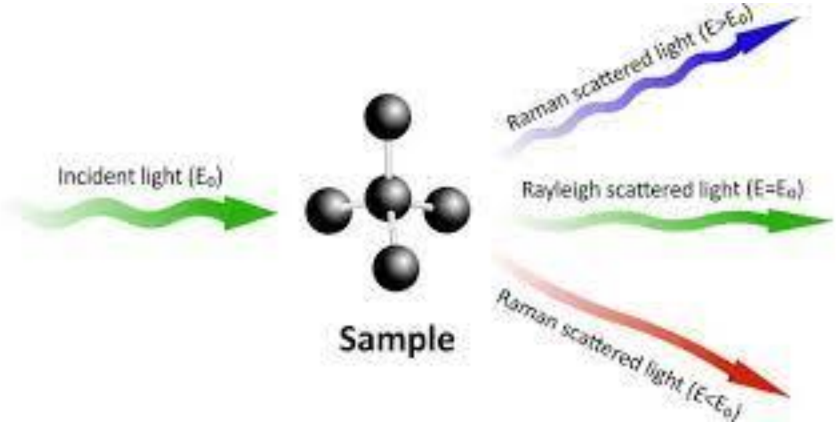
Scattering spectroscopy is a technique that involves the m**easurement of the scattered (dispersed) electromagnetic radiation by a sample.** It is used to study the interaction of light with matter, and provides information on the size, shape, and composition of particles in a sample. Scattering spectroscopy involves the measurement of the intensity and angular distribution of the scattered radiation, which is then used to identify the characteristics of the sample. Types:

Rayleigh scattering occurs when light is scattered by particles that are much smaller than the wavelength of the radiation, such as molecules in gases. It occurs in all directions and is responsible for the blue color of the sky.

Raman scattering occurs when incident radiation interacts with the vibrations of molecules in a sample, resulting in the emission of scattered radiation with different wavelengths. The Raman spectrum can be used to identify the types of molecules present in the sample, as different molecules will have unique Raman spectra.

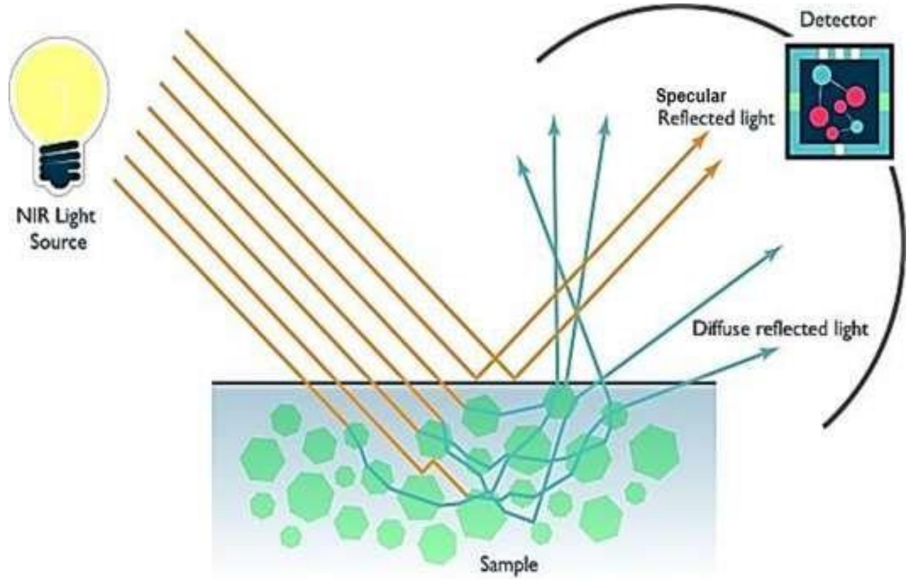
Dynamic light scattering is used to study the size and distribution of particles in a sample. It involves the measurement of the intensity and angular distribution of light scattered by particles suspended in a liquid. The scattering pattern is analyzed to determine the size distribution of the particles.





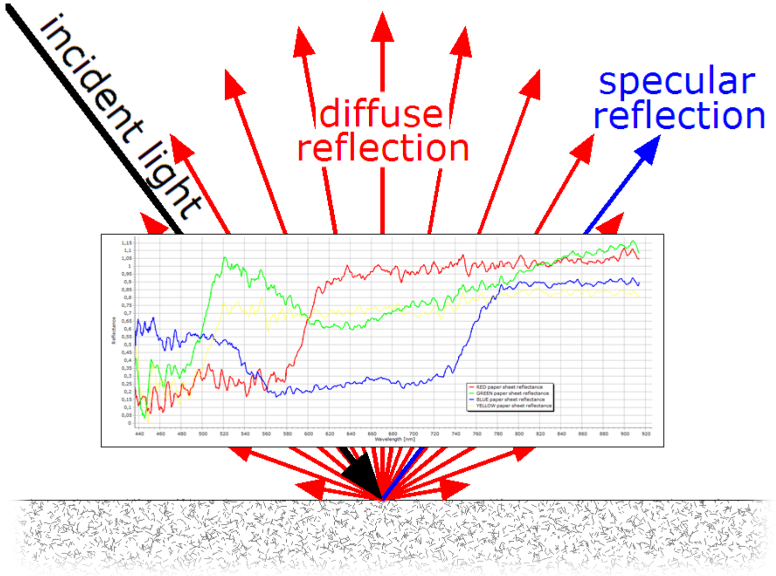
Reflection spectroscopy

Reflection spectroscopy is a technique used to analyze the behavior of light that is reflected off a material or surface. The technique is based on the measurement of the intensity of the **reflected light as a function of its wavelength or frequency**. Reflection spectroscopy can be used to determine the physical and chemical properties of a sample, such as its composition, thickness, and surface roughness.



There are several types of reflection spectroscopy, including infrared reflection spectroscopy, Raman reflection spectroscopy, and ultraviolet-visible reflection spectroscopy.

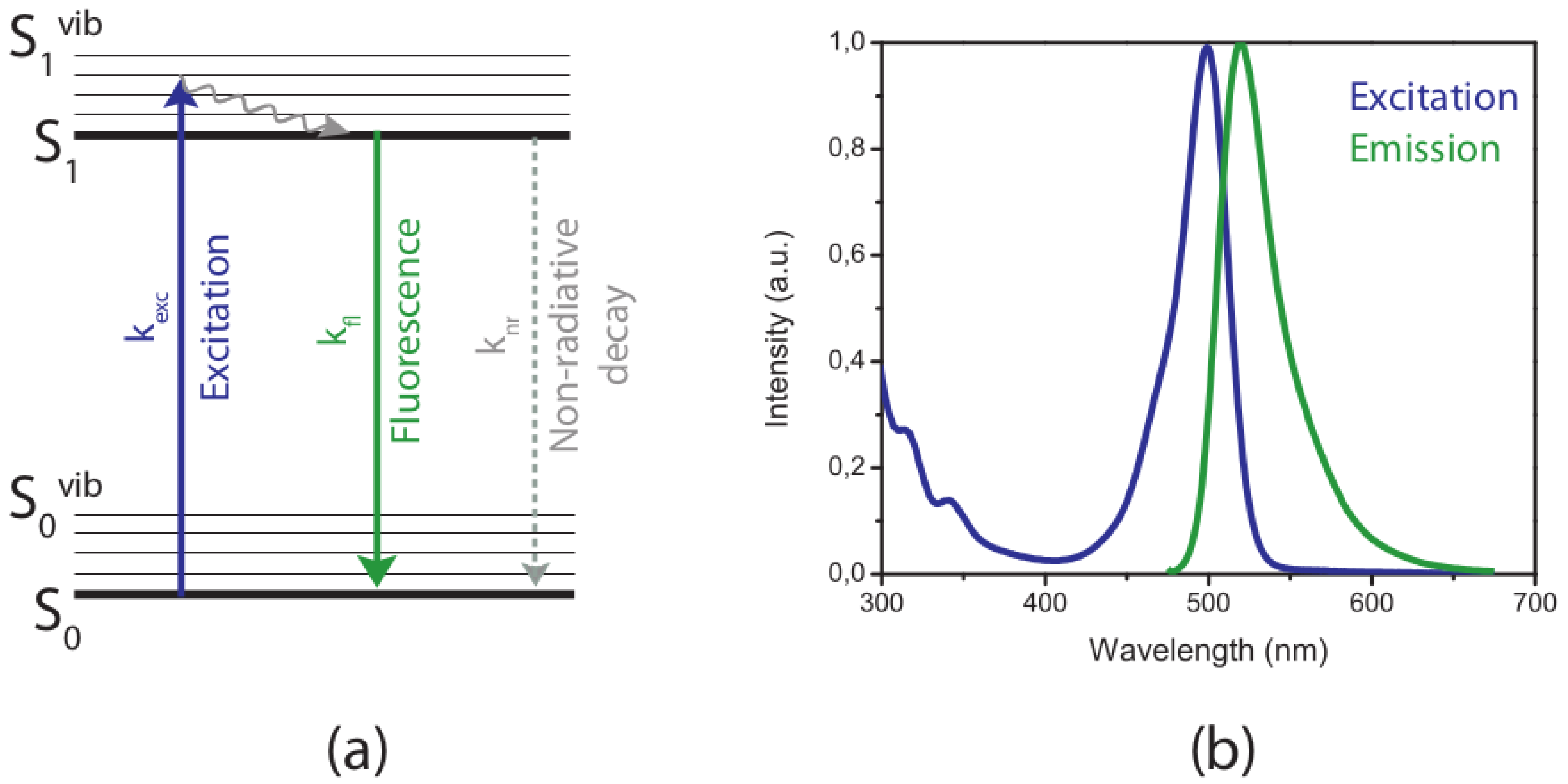
Infrared reflection spectroscopy is used to analyze the interaction of infrared radiation with a sample. It is commonly used in the analysis of solids and thin films to determine their chemical composition and structural properties.



Ultraviolet-visible (UV-Vis) reflection spectroscopy is used to measure the reflection of UV and visible light off a sample. It is commonly used to analyze thin films and coatings, and can provide information about the sample's optical properties.

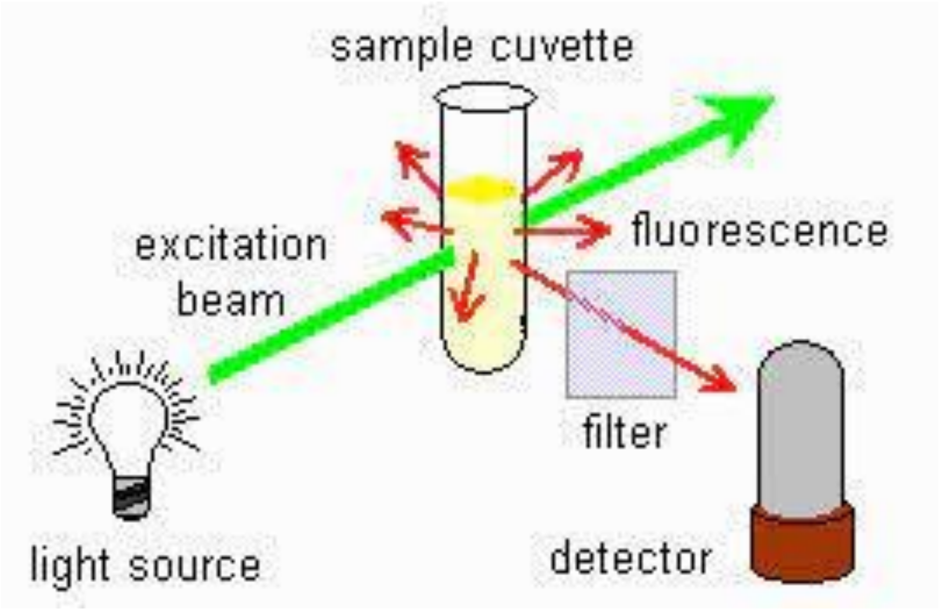
Fluorescence

Fluorescence is a phenomenon where a substance absorbs light of a particular wavelength and then emits light at a longer wavelength. This emission of light is usually at a lower energy level than the absorbed light. The emitted light is often of a different color than the absorbed light, and this property is used in various applications such as in fluorescence microscopy, forensics, and environmental monitoring. Fluorescence is caused by the excitation of electrons in the substance to a higher energy level, followed by their relaxation to a lower energy level and the release of light energy.

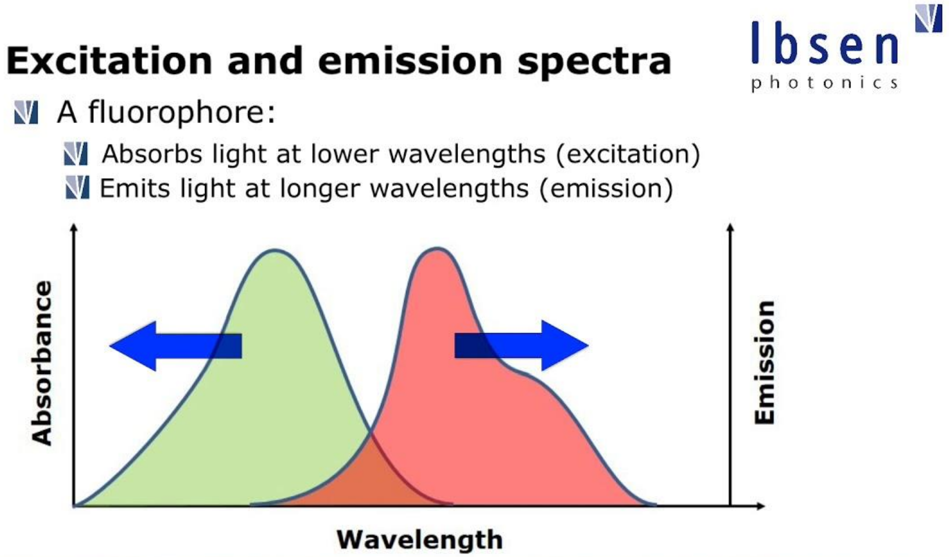


Fluorescence spectroscopy

Fluorescence spectroscopy is a technique used to measure the amount of light emitted by a sample when it is excited by a specific wavelength of light. The emitted light is called fluorescence, and the technique is used to study the properties and interactions of molecules. It is based on the principle that certain molecules absorb light energy at a specific wavelength and re-emit the energy as light at a longer wavelength.



Fluorescence spectroscopy involves shining light of a specific wavelength on a sample, which causes the electrons in the sample to become excited and jump to a higher energy level, or electronic state. The electrons then return to the original state and emit light of a longer wavelength. The emitted fluorescence can be measured and analyzed to obtain information about the properties of the sample.



Fluorescence spectroscopy is a sensitive technique, and many samples can be measured in very small amounts. Additionally, various forms of fluorescence spectroscopy, such as time-resolved fluorescence and fluorescence polarization, can provide additional information about the dynamics and structure of a sample.