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## Chapter 1 : Spectroscopy - Applications | calendrierdelascience.com

*Theory and Applications of Ultraviolet Spectroscopy. H. H. Jaffe and Milton Orchin. Wiley, New York, xv + pp. Illus. \$15 + See all authors and affiliations.*

Contributors Photoelectron spectroscopy involves the measurement of kinetic energy of photoelectrons to determine the binding energy, intensity and angular distributions of these electrons and use the information obtained to examine the electronic structure of molecules. Introduction Photoelectron spectroscopy PES is the energy measurements of photoelectrons emitted from solids, gases, or liquids by the photoelectric effect. The source of radiation for UPS is a noble gas discharge lamp, usually a He discharge lamp. Furthermore, depending on the source of the ionization energy, PES can probe either valence or core electrons. Photoelectric Effect To understand the principles of photoelectron spectroscopy, the photoelectric effect must be applied. The photoelectric effect states that electrons can be pushed off the surface of a solid by electromagnetic radiation. The ejected electrons are called photoelectrons. Scheme of photoelectric effect. Incoming light hits the surface of a solid causing the ejection of a photoelectron. Originally, known as the Hertz effect, the photoelectric effect was first observed by Heinrich Hertz in , when Hertz noticed that sparks would more readily jump between two charged surfaces that were illuminated with light. As PES can be used for energy measurements of solids, liquids, and gases the term photoionization or photoemission better represents the principles of PES. Photoionization is the process in which molecule M is ionized by a beam of photons, in which the molecule will lose an electron: The three-step model breaks down the process of photoionization into three independent steps: The excited electron will travel to the surface of the molecule. During this step, the excited electron travels it may or may not collide with other particles. Any excited electrons which do collide with a particle will loss energy. The excited electron will escape the surface of the molecule into the vacuum where it will be detected. The process of photoionization can only occur if the photon has energy greater than the energy which is holding the electron to the molecule, which is the lowest ionization potential. If there is excess energy after the ionization has occurred then the excess energy will be in the form of kinetic energy. These two variables, photon energy and kinetic energy, are both measured by the PE spectrometer. Thus, by using PES it is possible to measure the energies of the ground and excited states, after the loss of an electron from a neutral molecule, given by the above chemical formula. A basic photoionization process, showing the different ionization potentials. There are two types of ionization energy: Adiabatic ionization energy of a molecule is defined as the minimum amount of energy needed to eject an electron from the neutral molecule. Additionally, can be referred to as the difference between the energy of the vibrational ground state of the neutral molecule and positive ion. The vertical ionization energy is the most probable transition. The energy required to cause the ejection of an electron is known as ionization energy or electron binding energy. Overall, ionization energy will depend on the location of the electrons in preference to the nucleus of the molecule. As electrons are arranged in orbitals surrounding the atomic nucleus, the ionization energy will be higher or lower depending on whether the electrons are located in the core or valence shell. Obviously, core electrons, which are closer to the nucleus, will require more energy to be ejected. Furthermore, each chemical element has a different number of protons in the nucleus, resulting in a unique set of ionization energies for every element. By using photoelectron spectroscopy, the ionization energy is determined by subtracting the energy of the incoming photon from the measured kinetic energy of the ejected electron. The location of the ejected electron will factor greatly into which type of photoelectron spectroscopy is used. X-ray photoelectron spectroscopy XPS is used to eject electrons from the core or valence shell. The sample used in XPS will first be placed in an ultra-high vacuum chamber to prevent photons and emitted electrons from being absorbed by gases. Then the sample will be bombarded with x-rays, causing the ejection of electrons. The ejected electrons energies will be measured by their dispersal within an electric field. Due to the vacuum environment of the sample, XPS cannot be used for liquids. In addition, XPS will provide

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information about oxidation states for any elements present in the sample, as the ionization energies of core electrons are slightly higher when an oxidation state is present. UPS works in a similar fashion as XPS, but uses photons, produced by a noble gas discharge lamp, in the ultraviolet range of the spectrum. Originally, UPS was used only to determine the ionization energies of gaseous molecules; however, over the years it is also attributed information to the electronic structure of molecules. Splitting Various types of splitting occur in the photoelectron spectrum due to the removal of an electron from an orbital. The Russell-Saunders term symbol notation: In addition, spin orbit splitting will never occur for s orbitals, as it depends on an electron being removed from a degenerate subshell. The intensity of the peaks for the doublets will depend on the J value in the Russell-Saunders term. For example, the binding energy for the doublet with the lower J value will result in the highest intensity. Furthermore, due to nuclear shielding the magnitude of spin-orbit splitting will decrease the further the way from the nucleus. Another type of splitting is multiplet splitting which arises when there is interaction between an unpaired electron formed by photoelectron ejected and an already pre-existing unpaired electron. This can result in the formation of multiple final states being formed during the photoionization. For example, consider the three electron atom lithium. Photoelectron Instrumentation All photoelectron spectrometers must have three components. The first is an excitation source used to irradiate the sample into releasing electrons. The second is an electron energy analyzer which will disperse the emitted photoelectrons according to their respective kinetic energy. These various components in photoelectron spectrometers are available in many different forms, which are discussed within the module on Photoelectron Spectroscopy: A block diagram of a basic PE spectrometer is listed below: A block diagram of PE spectrometer. An example of a photoelectron spectrum obtained by a PE spectrometer is shown in Figure 5. This plot shows the kinetic energy distribution of emitted photon obtained by the electron energy analyzer, resulting in a plot of of the number of electrons detected versus the binding energy of electrons obtained. Describe how PES can be used to calculate the ionization energy of a molecule. Describe the photoelectric effect. Answers An X-ray radiation source. PES involves a given energy of photon to ionize a molecule. As the excess energy, will be in the form of kinetic energy, is calculated by the photoelectron spectrometer it is possible to calculate ionization energy of a molecule, by rearranging the following equation: The photoelectric effect occurs when light hits a metal surface; thus, causing the ejection of electrons from the surface of the metal.

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## Chapter 2 : Photoelectron Spectroscopy: Theory - Chemistry LibreTexts

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The basic parts of a spectrophotometer are a light source, a holder for the sample, a diffraction grating in a monochromator or a prism to separate the different wavelengths of light, and a detector. The detector is typically a photomultiplier tube, a photodiode, a photodiode array or a charge-coupled device CCD. Single photodiode detectors and photomultiplier tubes are used with scanning monochromators, which filter the light so that only light of a single wavelength reaches the detector at one time. The scanning monochromator moves the diffraction grating to "step-through" each wavelength so that its intensity may be measured as a function of wavelength. Fixed monochromators are used with CCDs and photodiode arrays. As both of these devices consist of many detectors grouped into one or two dimensional arrays, they are able to collect light of different wavelengths on different pixels or groups of pixels simultaneously. Simplified schematic of a double beam UV-visible spectrophotometer

A spectrophotometer can be either single beam or double beam. In a single beam instrument such as the Spectronic 20, all of the light passes through the sample cell. This was the earliest design and is still in common use in both teaching and industrial labs. In a double-beam instrument, the light is split into two beams before it reaches the sample. One beam is used as the reference; the other beam passes through the sample. Some double-beam instruments have two detectors photodiodes, and the sample and reference beam are measured at the same time. In other instruments, the two beams pass through a beam chopper, which blocks one beam at a time. The detector alternates between measuring the sample beam and the reference beam in synchronism with the chopper. There may also be one or more dark intervals in the chopper cycle. In this case, the measured beam intensities may be corrected by subtracting the intensity measured in the dark interval before the ratio is taken. In a single-beam instrument, the cuvette containing only a solvent has to be measured first. The light source consists of a Xenon flash lamp for the ultraviolet UV as well as for the visible VIS and near-infrared wavelength regions covering a spectral range from up to nm. The lamp flashes are focused on a glass fiber which drives the beam of light onto a cuvette containing the sample solution. The beam passes through the sample and specific wavelengths are absorbed by the sample components. The remaining light is collected after the cuvette by a glass fiber and driven into a spectrograph. The spectrograph consists of a diffraction grating that separates the light into the different wavelengths, and a CCD sensor to record the data, respectively. The whole spectrum is thus simultaneously measured, allowing for fast recording [10]. Samples are typically placed in a transparent cell, known as a cuvette. Test tubes can also be used as cuvettes in some instruments. The type of sample container used must allow radiation to pass over the spectral region of interest. The most widely applicable cuvettes are made of high quality fused silica or quartz glass because these are transparent throughout the UV, visible and near infrared regions. Glass and plastic cuvettes are also common, although glass and most plastics absorb in the UV, which limits their usefulness to visible wavelengths. These include attaching spectrophotometers to telescopes to measure the spectra of astronomical features. UV-visible microspectrophotometers consist of a UV-visible microscope integrated with a UV-visible spectrophotometer. A complete spectrum of the absorption at all wavelengths of interest can often be produced directly by a more sophisticated spectrophotometer. In simpler instruments the absorption is determined one wavelength at a time and then compiled into a spectrum by the operator. Microspectrophotometry[ edit ] UV-visible spectroscopy of microscopic samples is done by integrating an optical microscope with UV-visible optics, white light sources, a monochromator, and a sensitive detector such as a charge-coupled device CCD or photomultiplier tube PMT. As only a single optical path is available, these are single beam instruments. Modern instruments are capable of measuring UV-visible spectra in both reflectance and transmission of micron-scale sampling areas. The advantages of using such instruments is that they are able to measure microscopic samples but are also able to measure the

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spectra of larger samples with high spatial resolution. As such, they are used in the forensic laboratory to analyze the dyes and pigments in individual textile fibers, [11] microscopic paint chips [12] and the color of glass fragments. They are also used in materials science and biological research and for determining the energy content of coal and petroleum source rock by measuring the vitrinite reflectance. Microspectrophotometers are used in the semiconductor and micro-optics industries for monitoring the thickness of thin films after they have been deposited. In the semiconductor industry, they are used because the critical dimensions of circuitry is microscopic. A typical test of a semiconductor wafer would entail the acquisition of spectra from many points on a patterned or unpatterned wafer. The thickness of the deposited films may be calculated from the interference pattern of the spectra. In addition, ultraviolet-visible spectrophotometry can be used to determine the thickness, along with the refractive index and extinction coefficient of thin films as described in Refractive index and extinction coefficient of thin film materials. A map of the film thickness across the entire wafer can then be generated and used for quality control purposes. From these measurements, the concentration of the two species can be calculated. Therefore, graphing the natural log  $\ln$  of the concentration  $[A]$  versus time will graph a line with slope  $-k$ , or negative the rate constant. Different rate orders have different integrated rate laws depending on the mechanism of the reaction. After determining optimal wavelengths for all species involved in equilibria, a reaction can be run to equilibrium, and the concentration of species determined from spectroscopy at various known wavelengths. See also [edit] Isosbestic point important in kinetics measurements. A wavelength where absorption does not change as the reaction proceeds.

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## Chapter 3 : Spectroscopy - Wikipedia

*The other name of UV (Ultra-Violet) spectroscopy is Electronic spectroscopy as it involves the promotion of the electrons from the ground state to the higher energy or excited state. In this article I will explain the basic principle, working and all the applications of UV spectroscopy.*

Contributors Photoelectron spectroscopy PES is a technique used for determining the ionization potentials of molecules. Underneath the banner of PES are two separate techniques for quantitative and qualitative measurements. UPS focuses on ionization of valence electrons while XPS is able to go a step further and ionize core electrons and pry them away. The key point in PES is that a lot of qualitative and quantitative information can be learned about the surface region of solids. There are a few basics common to both techniques that must always be present in the instrumental setup. The radiation sources used in PES are fixed-energy radiation sources. PES analyzers are various types of electron energy analyzers A high vacuum environment: PES is rather picky when it comes to keeping the surface of the sample clean and keeping the rest of the environment free of interferences from things like gas molecules. The high vacuum is almost always an ultra high vacuum UHV environment. When the sample is irradiated, the released photoelectrons pass through the lens system which slows them down before they enter the energy analyzer. The analyzer shown is a spherical deflection analyzer which the photoelectrons pass through before they are collected at the collector slit. For a more versatile light source, synchrotron radiation sources are also used. The main thing to consider when choosing a radiation source is the kinetic energy involved. The source is what sets the kinetic energy of the photoelectrons, so there needs to not only be enough energy present to cause the ionizations, but there must also be an analyzer capable of measuring the kinetic energy of the released photoelectrons. In XPS experiments, electron guns can also be used in conjunction with x-rays to eject photoelectrons. There are a couple of advantages and disadvantages to doing this, however. With an electron gun, the electron beam is easily focused and the excitation of photoelectrons can be constantly varied. Unfortunately, the background radiation is increased significantly due to the scattering of falling electrons. Also, a good portion of substances that are of any experimental interest are actually decomposed by heavy electron bombardment such as that coming from an electron gun. Analyzers There are two main classes of analyzers well-suited for PES - kinetic energy analyzers and deflection or electrostatic analyzers. The intensity of the spectra produced is also dependent on the kinetic energy. The faster the electrons are moving, the lower the resolution and intensity is. In order to actually get well resolved, useful data other components must be introduced into the instrument. Adding a system of optics lenses to a PES instrument helps with this problem immensely. Electron optics are capable of decelerating the photoelectrons through retardation of the electric field. The energy the photoelectrons decelerate to is known as the "pass energy. Optics are also capable of accelerating the electrons as well. The design of any lens system greatly effects the photoelectron counts. These lenses are also capable of focusing on a small area of a particular sample. Specific Analyzers Within the broad picture of two main analyzer classes, there are a variety of specific analyzers in existence that are used in PES. The list below goes over several well-used analyzers, though this list is, by no means, exhaustive. The most common type of analyzer is a hemispherical analyzer, which will be explained in more depth under the spherical deflection analyzer topic. These analyzers are condensers made from two parallel plates with a distance,  $d$ , across them. Parabolic trajectories of electrons are obtained due to the constant potential difference,  $V$ , between the two plates. Schematic of a PMA where the angle between the bottom plate and the electrons entering is 45 degrees and the angle between the bottom plate and the electrons exiting is also 45 degrees. In order for transmission to occur, the potential must be: To obtain better focus, the electron entrance and exit angle is capable of being shifted to 30 degrees, but this is not necessarily a good idea as it sacrifices transmission instead. The entrance and exit slits are all contained on the inner cylinder. Schematic of a CMA where the angle between the center of the cylinders and the electrons is  $\theta$ .  $R_{in}$  is the radius of the inner cylinder and  $R_{out}$  is the radius of the outer

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cylinder. The electron path should be more parabolic than the overly elliptical shape shown here. They are good for applications that require a high sensitivity with only a moderate resolution. It is this reason that CDAs are sometimes called "degree analyzers. Schematic of a CDA where the angle the cylinders span is degrees. These analyzers have high resolution, however their transmission is low. Schematic of an SDA. Only photoelectrons of the correct energy are able to pass through the detector with the right arc and exit instead of colliding with the side walls of the hemispheres and becoming lost. Here, the potential is different for both the inner and the outer hemisphere: For this to occur, the analyzer is also arranged so that only photoelectrons of a specific, fixed kinetic energy will pass through and reach the detector. In this case, the lens is scanned for different energies. The hemispheres of the analyzer here have a potential difference between them that is varied so that photoelectrons of different kinetic energies can reach the detector. The more common of these two modes is FAT because it provides a greater signal intensity at low electron kinetic energy and is also makes quantification of the spectra simpler. These analyzers are a particularly good class of deflection analyzer. The photoelectrons that do make it through the entrance slits will then only exit if they follow a specific, curved path down the middle of the two hemispheres. The path they follow has the "correct energy" for exit to occur, and is determined by the selection of  $V_{in}$  and  $V_{out}$ . Photoelectrons that are of higher or lower kinetic energy than what is defined by the hemispheres will be lost through collisions with the walls. One type of energy measured is the binding energy, which is calculated through the following equation: These devices act as electron amplifiers because they are coated with a material that produce secondary photoelectrons when they are struck by an electron. Typically, they are able to produce two to three photoelectrons per every electron they are hit with. One type of spectra in these experiments is recorded by varying the potential difference between the plates or hemispheres of the analyzer. The output is known as an electron kinetic energy spectrum and is obtained by measuring the photoelectron current at the detector as a function of the voltage applied to the hemispheres or plates. The voltage is then used in the calculation of kinetic energy. The problems in resolution come from four main areas: Steps can be taken to improve the resolution, but some methods then sacrifice other factors such as the sensitivity. Obtaining high spatial resolution and high energy resolution always comes at the expense of the signal intensity. For example, in an SDA these slits are what define the range of trajectories photoelectrons may have when entering or exiting the analyzer. Decreasing the widths will certainly cause the resolution to go up, but the smaller slit size will decrease the number of photoelectrons allowed in and out of the analyzer, therefore lowering the sensitivity. A third method of improving resolution is specific to XPS and is the addition of an x-ray monochromator to the system. The use of monochromatic x-rays also serves to simplify the spectrum. The photoelectrons produced are passed through a slit into a vacuum region where they are then deflected by magnetic or electrostatic fields to give an energy spectrum. As in figure 1 at the start of this module, the analyzer in use is an SDA. In this instrument, there are no optics in use, nor is there an electron multiplier. This schematic shows separate chambers for the sample and the analyzer, both of which are under UHV. There are two main areas UPS is used to study: Electronic structure of solids 2. The measurement of molecular orbital energies that can be compared to theoretical values calculated from quantum chemistry 2. The binding and orientation of adsorbed species on the surface of solids 4. These also correspond to the orbital energies. Advantages Ultraviolet radiation has a very narrow line width and a high flux of photons available from simple discharge sources. This is because the kinetic energy of the escaping photoelectrons limits the depth able to be probed. The samples studied are all solids of some type ranging from metals to frozen liquids. When the sample is irradiated, the electrons ejected are from the inner shells of the atoms. There are several areas suited to measurement by XPS:

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## Chapter 4 : calendrierdelascience.com: Customer reviews: Theory and Applications of Ultraviolet Spectroscopy

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Principle, working and applications of UV spectroscopy Posted Date: Aman Thakur Member Level: The other name of UV Ultra-Violet spectroscopy is Electronic spectroscopy as it involves the promotion of the electrons from the ground state to the higher energy or excited state. In this article I will explain the basic principle, working and all the applications of UV spectroscopy. Introduction to UV spectroscopy UV spectroscopy is type of absorption spectroscopy in which light of ultra-violet region nm. Absorption of the ultra-violet radiations results in the excitation of the electrons from the ground state to higher energy state. For most of the molecules, the lowest energy occupied molecular orbitals are s orbital, which correspond to sigma bonds. The p orbitals are at somewhat higher energy levels, the orbitals nonbonding orbitals with unshared paired of electrons lie at higher energy levels. In all the compounds other than alkanes, the electrons undergo various transitions. Some of the important transitions with increasing energies are: This is the basic principle of UV spectroscopy. Instrumentation and working of UV spectroscopy Instrumentation and working of the UV spectrometers can be studied simultaneously. Most of the modern UV spectrometers consist of the following parts- Light Source- Tungsten filament lamps and Hydrogen-Deuterium lamps are most widely used and suitable light source as they cover the whole UV region. Tungsten filament lamps are rich in red radiations; more specifically they emit the radiations of nm, while the intensity of Hydrogen-Deuterium lamps falls below nm. Monochromator- Monochromators generally composed of prisms and slits. The most of the spectrophotometers are double beam spectrophotometers. The radiation emitted from the primary source is dispersed with the help of rotating prisms. The various wavelengths of the light source which are separated by the prism are then selected by the slits such the rotation of the prism results in a series of continuously increasing wavelength to pass through the slits for recording purpose. The beam selected by the slit is monochromatic and further divided into two beams with the help of another prism. Both sample and reference solution are contained in the cells. These cells are made of either silica or quartz. Detector- Generally two photocells serve the purpose of detector in UV spectroscopy. One of the photocell receives the beam from sample cell and second detector receives the beam from the reference. The intensity of the radiation from the reference cell is stronger than the beam of sample cell. This results in the generation of pulsating or alternating currents in the photocells. Amplifier- The alternating current generated in the photocells is transferred to the amplifier. The amplifier is coupled to a small servometer. Generally current generated in the photocells is of very low intensity, the main purpose of amplifier is to amplify the signals many times so we can get clear and recordable signals. Recording devices- Most of the time amplifier is coupled to a pen recorder which is connected to the computer. Computer stores all the data generated and produces the spectrum of the desired compound. Concept of Chromophore and Auxochrome in the UV spectroscopy Chromophore- Chromophore is defined as any isolated covalently bonded group that shows a characteristic absorption in the ultraviolet or visible region nm. Ethylenes and acetylenes are the example of such chromophores. Carbonyl, nitriles, azo compounds, nitro compounds etc. Auxochromes- An auxochrome can be defined as any group which does not itself act as a chromophore but whose presence brings about a shift of the absorption band towards the longer wavelength of the spectrum. Absorption and intensity shifts in the UV spectroscopy There are four types of shifts observed in the UV spectroscopy- a Bathochromic effect- This type of shift is also known as red shift. Bathochromic shift is an effect by virtue of which the absorption maximum is shifted towards the longer wavelength due to the presence of an auxochrome or change in solvents. Hypsochromic shift is an effect by virtue of which absorption maximum is shifted towards the shorter wavelength. Generally it is caused due to the removal of conjugation or by changing the polarity of the solvents. The introduction of an auxochrome in

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the compound generally results in the hyperchromic effect. Hyperchromic effect occurs due to the distortion of the geometry of the molecule with an introduction of new group. Applications of UV spectroscopy

1. Detection of functional groups- UV spectroscopy is used to detect the presence or absence of chromophore in the compound. This is technique is not useful for the detection of chromophore in complex compounds. The absence of a band at a particular band can be seen as an evidence for the absence of a particular group. If the spectrum of a compound comes out to be transparent above nm than it confirms the absence of  $\pi$  conjugation
2. A carbonyl group
3. Benzene or aromatic compound
4. Bromo or iodo atoms.

Detection of extent of conjugation- The extent of conjugation in the polyenes can be detected with the help of UV spectroscopy. With the increase in double bonds the absorption shifts towards the longer wavelength. If the double bond is increased by 8 in the polyenes then that polyene appears visible to the human eye as the absorption comes in the visible region.

Identification of an unknown compound- An unknown compound can be identified with the help of UV spectroscopy. The spectrum of unknown compound is compared with the spectrum of a reference compound and if both the spectrums coincide then it confirms the identification of the unknown substance.

Determination of configurations of geometrical isomers- It is observed that cis-alkenes absorb at different wavelength than the trans-alkenes. The two isomers can be distinguished with each other when one of the isomers has non-coplanar structure due to steric hindrances. The cis-isomer suffers distortion and absorbs at lower wavelength as compared to trans-isomer.

Determination of the purity of a substance- Purity of a substance can also be determined with the help of UV spectroscopy. The absorption of the sample solution is compared with the absorption of the reference solution. The intensity of the absorption can be used for the relative calculation of the purity of the sample substance.

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## Chapter 5 : Ultraviolet-visible spectroscopy - Wikipedia

*Ultraviolet-visible spectroscopy or ultraviolet-visible spectrophotometry (UV-Vis or UV/Vis) refers to absorption spectroscopy or reflectance spectroscopy in the ultraviolet-visible spectral region. This means it uses light in the visible and adjacent ranges.*

Applications Spectroscopy is used as a tool for studying the structures of atoms and molecules. The large number of wavelengths emitted by these systems makes it possible to investigate their structures in detail, including the electron configurations of ground and various excited states. Spectroscopy also provides a precise analytical method for finding the constituents in material having unknown chemical composition. In a typical spectroscopic analysis, a concentration of a few parts per million of a trace element in a material can be detected through its emission spectrum. In astronomy the study of the spectral emission lines of distant galaxies led to the discovery that the universe is expanding rapidly and isotropically independent of direction. The finding was based on the observation of a Doppler shift of spectral lines. The Doppler shift is an effect that occurs when a source of radiation such as a star moves relative to an observer. The frequency will be shifted in much the same way that an observer on a moving train hears a shift in the frequency of the pitch of a ringing bell at a railroad crossing. The pitch of the bell sounds higher if the train is approaching the crossing and lower if it is moving away. Similarly, light frequencies will be Doppler-shifted up or down depending on whether the light source is approaching or receding from the observer. During the 1920s, the American astronomer Edwin Hubble identified the diffuse elliptical and spiral objects that had been observed as galaxies. He went on to discover and measure a roughly linear relationship between the distance of these galaxies from Earth and their Doppler shift. In any direction one looks, the farther the galaxy appears, the faster it is receding from Earth. Spectroscopic evidence that the universe was expanding was followed by the discovery in 1965 of a low level of isotropic microwave radiation by the American scientists Arno A. Penzias and Robert W. Wilson. The measured spectrum is identical to the radiation distribution expected from a blackbody, a surface that can absorb all the radiation incident on it. This radiation, which is currently at a temperature of 2.7 K, is called the cosmic microwave background. Practical considerations General methods of spectroscopy Production and analysis of a spectrum usually require the following: The apparatus used to accept light, separate it into its component wavelengths, and detect the spectrum is called a spectrometer. Spectra can be obtained either in the form of emission spectra, which show one or more bright lines or bands on a dark background, or absorption spectra, which have a continuously bright background except for one or more dark lines. Absorption spectroscopy measures the loss of electromagnetic energy after it illuminates the sample under study. For example, if a light source with a broad band of wavelengths is directed at a vapour of atoms, ions, or molecules, the particles will absorb those wavelengths that can excite them from one quantum state to another. As a result, the absorbed wavelengths will be missing from the original light spectrum after it has passed through the sample. Since most atoms and many molecules have unique and identifiable energy levels, a measurement of the missing absorption lines allows identification of the absorbing species. Absorption within a continuous band of wavelengths is also possible. This is particularly common when there is a high density of absorption lines that have been broadened by strong perturbations by surrounding atoms. In the laboratory environment, transparent chambers or containers with windows at both ends serve as absorption cells for the production of absorption spectra. Light with a continuous distribution of wavelength is passed through the cell. When a gas or vapour is introduced, the change in the transmitted spectrum gives the absorption spectrum of the gas. Often, absorption cells are enclosed in ovens because many materials of spectroscopic interest vaporize significantly only at high temperatures. In other cases, the sample to be studied need not be contained at all. For example, interstellar molecules can be detected by studying the absorption of the radiation from a background star. The absorption of ultraviolet and X-ray radiation by the upper atmosphere prevents this harmful portion of the electromagnetic spectrum from irradiating the inhabitants of Earth. The fact that water vapour, carbon dioxide

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, and other gases reflect infrared radiation is important in determining how much heat from Earth is radiated into space. This phenomenon is known as the greenhouse effect since it works in much the same way as the glass panes of a greenhouse; that is to say, energy in the form of visible light is allowed to pass through the glass, while heat in the form of infrared radiation is absorbed and reflected back by it, thus keeping the greenhouse warm. Similarly, the transmission characteristics of the atmosphere are important factors in determining the global temperature of Earth. The second main type of spectroscopy, emission spectroscopy, uses some means to excite the sample of interest. In its use as an analytical tool, this fluorescence radiation is the complement of the missing wavelengths in absorption spectroscopy. Early excitation methods included placing the sample in a flame or an electric-arc discharge. The atoms or molecules were excited by collisions with electrons, the broadband light in the excitation source, or collisions with energetic atoms. The analysis of the emission lines is done with the same types of spectrometer as used in absorption spectroscopy.

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## Chapter 6 : Photoelectron Spectroscopy: Application - Chemistry LibreTexts

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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. The various implementations and techniques can be classified in several ways. Type of radiative energy[ edit ] This section does not cite any sources. Please help improve this section by adding citations to reliable sources. Unsourced material may be challenged and removed. June Learn how and when to remove this template message The types of spectroscopy are distinguished by the type of radiative energy involved in the interaction. In many applications, the spectrum is determined by measuring changes in the intensity or frequency of this energy. The types of radiative energy studied include: Electromagnetic radiation was the first source of energy used for spectroscopic studies. Techniques that employ electromagnetic radiation are typically classified by the wavelength region of the spectrum and include microwave, terahertz, infrared, near-infrared, ultraviolet-visible, x-ray, and gamma spectroscopy. Particles, because of their de Broglie waves, can also be a source of radiative energy. Both electron and neutron spectroscopy are commonly used. For a particle, its kinetic energy determines its wavelength. Acoustic spectroscopy involves radiated pressure waves. Dynamic mechanical analysis can be employed to impart radiating energy, similar to acoustic waves, to solid materials. Nature of the interaction[ edit ] The types of spectroscopy also can be distinguished by the nature of the interaction between the energy and the material. Absorption occurs when energy from the radiative source is absorbed by the material. Absorption is often determined by measuring the fraction of energy transmitted through the material, with absorption decreasing the transmitted portion. Emission indicates that radiative energy is released by the material. This feature can be measured in the infrared by instruments such as the atmospheric emitted radiance interferometer. Elastic scattering and reflection spectroscopy determine how incident radiation is reflected or scattered by a material. Crystallography employs the scattering of high energy radiation, such as x-rays and electrons, to examine the arrangement of atoms in proteins and solid crystals. Impedance is the ability of a medium to impede or slow the transmittance of energy. For optical applications, this is characterized by the index of refraction. Inelastic scattering phenomena involve an exchange of energy between the radiation and the matter that shifts the wavelength of the scattered radiation. These include Raman and Compton scattering. Coherent or resonance spectroscopy are techniques where the radiative energy couples two quantum states of the material in a coherent interaction that is sustained by the radiating field. The coherence can be disrupted by other interactions, such as particle collisions and energy transfer, and so often require high intensity radiation to be sustained. Nuclear magnetic resonance NMR spectroscopy is a widely used resonance method, and ultrafast laser spectroscopy is also possible in the infrared and visible spectral regions. Type of material[ edit ] This section does not cite any sources.

## Chapter 7 : Theory and applications of ultraviolet spectroscopy (Book, ) [calendrierdelascience.com]

*Basic UV-Vis Theory, Concepts and Applications Page 1 of 28 Introduction Ultraviolet and visible spectrometers have*

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*been in general use for the last 35 years and over this period have become the most.*

## Chapter 8 : Principle, working and applications of UV spectroscopy

*Theory and Applications of Ultraviolet Spectroscopy. H. H. Jaffe and Milton Orchin. Wiley, New York, xv + pp. Illus. \$15  
Theory and Applications of.*