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Spectroscopic Measurements as Scientific Tool

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Abstract

This paper is an attempt to introduce the Spectroscopic measurement techniques in simple form. It covers the meaning of 'Spectroscopy' in general and infrared, visible and ultra-violet spectroscopy in particular. The instruments and techniques involved to observe and analyze different spectrum are highlighted under emission spectroscopy and absorption spectroscopy. Finally, the application of spectrographic methods in various fields of science like chemistry, physics, astronomy, biology and medicine, food science, metallurgy and forensic science are discussed in brief without going into any technical complexities.

Introduction

The milestones crossed by scientists through the 'spectroscope' form numerous list of applications not only to a research scientist but also it finds day-to-day application and increasing use in technological laboratories. The technological laboratories that make use of this include factories, mines, crime-detection bureaus, public health departments, hospitals, museums and technical research institutes. On the

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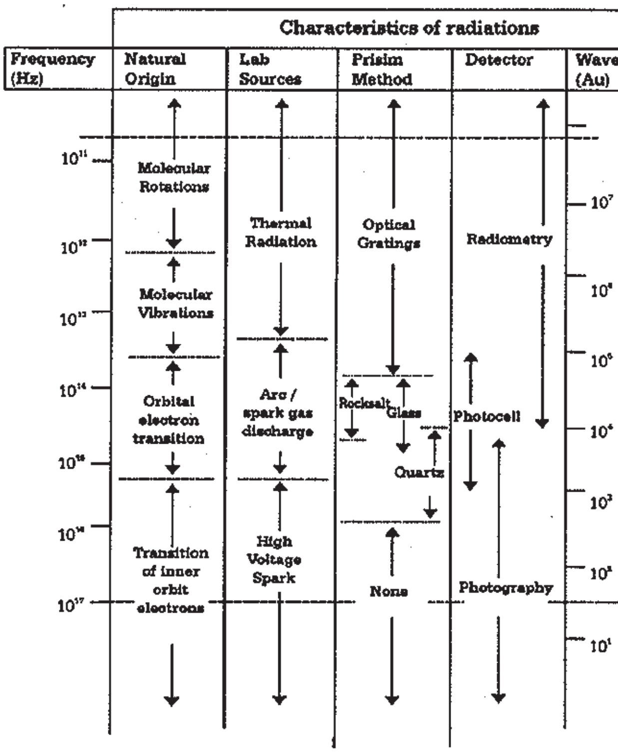
other hand, this has achieved the status of most powerful instrument in investigating the natural universe. The objective of the essay is to highlight the various applications of Spectroscopy in general and spectroscopic measurements in particular.

Spectroscopy is the study of electromagnetic radiations. A spectrum is the ordered arrangement of electromagnetic radiations in the order of increasing frequency or decreasing wavelength. The wavelength of several thousand Km up to trillionth of a millimeter covers this spectrum. The electromagnetic spectrum is divided into various 'Regions' in accordance with the types of instruments available to produce and detect these waves of varied lengths. It lists up the Radio waves, Infrared radiation, visible light, Ultra-violet rays, X-rays, g-rays and Cosmic rays in the order of increasing frequency or energy.

In this paper we limit the term 'Spectroscopy' to the study of those radiations covered under Infrared, visible and ultra-violet regions only. These regions, its ranges and properties of these regions are summarized in Table 1.

Table 1:

The Spectroscopic part of the electromagnetic spectrum



In 1666, Sir Isaac Newton obtained the spectrum of visible light by inserting a glass prism along the path of a beam of sunlight.

W.H. Wollaston improved this further in 1802 and by Fraunhofer in 1834. The credit of designing first ever practical spectroscope goes to G.R. Kirchoff and R. Bunsen in the year 1859. The spectroscope developed by them was then useful for qualitative chemical analysis. They could discover several elements and they were able to detect the presence of many known elements in Sun. So they are the founders of Modern Spectroscopy in real sense. Different spectroscopic techniques are used now a days to detect different ranges of 'Spectroscopy' under study.

Infrared Spectrum

Coarse Diffraction gratings or prisms of Rocksalt, which are transparent to longer waves than in glass, can disperse the infrared radiations. These are detectable by Bolometer, Thermocouples, and similar Radiometers. Globar heaters and similar incandescent heaters can emit infrared radiations. Infrared spectrum extends from the edge of visible spectrum up to about 1 mm. It has assumed great importance in chemical and biological research because of the highly specific absorption of chemical compounds at these wavelengths. It is called 'molecular fingerprint'.

Visible Spectrum

The spectral region sensitive to eye is visible spectrum. They lie in the wavelength region of 4000 Au to 7500 Au. This region is used in visual spectroscopy and colorimetric analysis. Apart from the fact that this region is sensitive to optic nerve, they are also characterized by deviation when passed through prisms and gratings. They can be photographed and measurements are comparatively easier with the use of photocells.

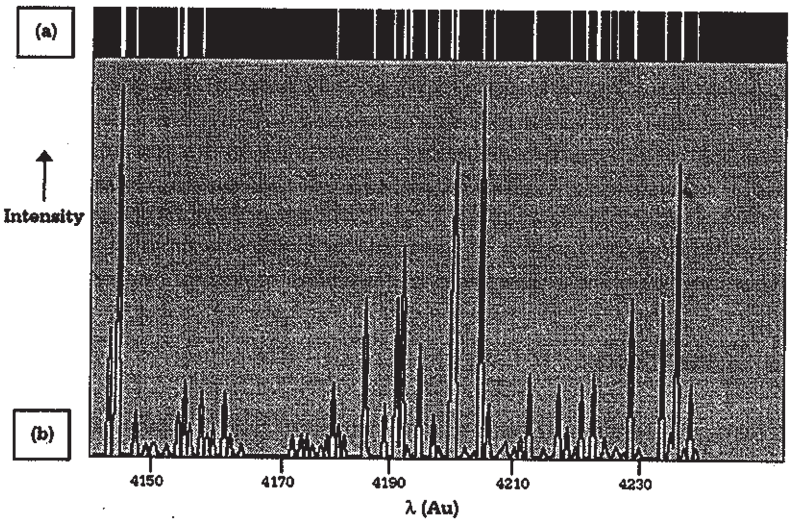
Ultraviolet Spectrum

This spectrum ranges from nearly 3000 Au and goes down to 10 Au (nearing X-ray region). Ordinary glass is not transparent to

ultra-violet region. Quartz, Fluorite, Rocksalt, Water etc., are highly transparent to ultra-violet region. This region is of great importance in absorption spectrophotometry and in the analysis of materials by emission spectrum. It forms one of the richest and most useful regions of the spectrum.

The Spectroscope and Spectrograph

Any device used to observe the spectrum is a Spectroscope. The instrument, which produces the photographic record of spectrum, is Spectrograph. The spectral lines are detected or recorded by different methods. Infrared spectrographs have Radiometer, which record the variation in current through galvanometer. Photographic method is more sensitive method in the region 10 Au to 15000 Au. Densitometer records of spectrographs are highly useful in quantitative analysis. Diagrams (a) and (b) give the idea of photographic record and photoelectric record of typical iron spectrum in near violet region.



(a) Photographic and (b) photoelectric records of spectrum of iron

Techniques adopted in Spectroscopy

Two techniques are adopted in spectroscopy: Emission spectroscopy and Absorption spectroscopy.

Emission spectroscopy

Spectrum emitted due to various physical conditions of atoms and molecules is emission spectroscopy. Three kinds of emission spectra are identifiable. The are Line, Band and Continuous Spectra.

Line spectra are due to atomic gases or irons when heated to incandescence.

Band Spectra originates from molecules like polyatomic incandescent gases and vapour.

Continuous spectra result from light radiated by incandescent solids and liquids. It is overlapped version of line and Band spectra.

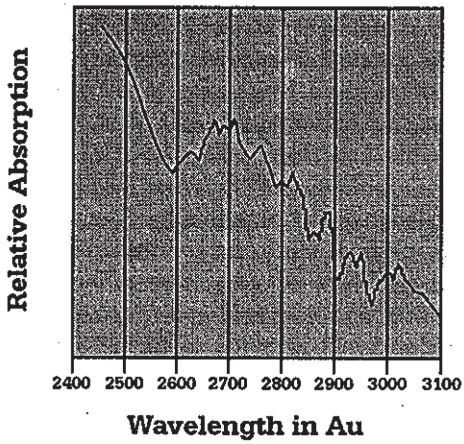
Each atom or molecule produces a characteristic set of spectrum lines or bands, which is its 'finger print' as mentioned earlier. Hence, the study of the spectrum of a material, be it an alloy, compound in a laboratory, or a star or nebula – gives the characteristic property of the same. Measurement of wavelengths of special lines can be done to the precision of one in several million. Further each atom emits many characteristics spectral lines. Hence the study of 'spectrum' of a material can identify the several atoms it is made up of. However, the drawback of the method is, it cannot be directly applied to detect molecules because most of the molecules get dissociated in electric arc or spark. (Arc/spark process is a must to get the spectrum.) Further, the negative radicals are not detectable by this method. Elements like sulphur, selenium, chloride, bromide, iodine, etc., require special spectroscopic technique, which are more complicated than other methods of chemical analysis.

Emission spectroscopic method is also useful in quantitative analysis of materials. At very low concentration of elements in a material, the intensity characteristics of spectral lines emitted by that element is directly proportional to number of atoms in that material. This linearity provides the basis for quantitative analysis of materials. Such quantitative analysis is possible for over seventy elements of periodic table – which are rapid and accurate. Further, very small quantity of material is sufficient to detect and measure all the elements unlike 'wet methods'. As small as 10 mg of sample is sufficient to detect all the 70 elements.

Analysis by emission spectra normally called spectrochemical analysis is widely used in industry for determining the constituents of alloys, impurities, etc., and for testing of biological, medical and food products.

Absorption Spectroscopy

When a spectrum of light is observed through a coloured glass, certain wavelengths exhibit reduced intensity due to absorption. This absorption is also found in infrared and ultra violet region of spectrum lines. Solids in solution and liquids can exhibit this property of absorption. This is absorption spectrum. A spectroscopic study of this type has two broad aims – To know which are the wavelengths absorbed and by how much. Hence the absorption spectroscopy can serve as 'finger print' of chemical substance in liquid form – for which emission spectroscopy has limitation due to dissociation in arc/spark. Absorption spectrophotometry is the technique used for quantitative absorption spectroscopy. It can be used for quantitative analysis of organic molecules like analysis of vitamins, hormones and dyes concentration, etc. By the study of absorption photograph of the molecules, a curve may be established as shown in Diagram C.



Intensity of absorption of various characteristic wavelengths for a given thickness of solution can be measured by spectrophotometric methods – which gives the concentration of the elements.

Fluorescence spectroscopy is a recent development in absorption spectroscopy. Here, the object to be studied is shielded from extraneous light and illuminated light by ultra violet light from a Hg – lamp and a filter to absorb visible radiation. The spectrum glows due to fluorescence. The wavelengths of this glow determine the characteristics of the specimen. Normally, this spectroscopy is applied in mineralogy, biochemistry, biology, medicine and food industry.

Many organic materials produce fluorescence. Certain species of bacteria have the fluorescence characteristic. Bacteria growth on meat can be detected by their fluorescence. Mineral oils, unlike the most of organic oils have fluorescent property – used widely in detection of contamination of mineral oils with organic oils. Real and artificial gems can be distinguished by the study of fluorescence spectroscopy.

Spectroscopy in different fields of science

The discussion of the uses of spectroscopy would be an endless effort. In the present frame, we may limit the same to discuss its uses in natural sciences like chemistry, physics, astronomy, biology and medicine, food research, metallurgy and forensic sciences.

Spectroscopy in Chemistry

Many chemical elements like Cesium, Rubidium, Helium, Gallium, Indium, Thallium, etc., were discovered by spectroscopic methods, soon Kirchoff and Bunsen developed the practical spectroscope in 1859.

In later years, the application of spectroscopic methods grew powerful with time and led to the discovery of rare isotopes of Carbon, Nitrogen and Oxygen. The contribution of spectroscopy to chemistry is not just limited to the field of discovery of elements. It is useful in finding the structure of many molecules by the study of their spectra. Structures of penicillin and Vitamin K were worked out with extensive help of spectroscope.

Spectroscopy is used as a tool to measure the strength of chemical bonds in compounds and also the equilibrium constants to a very high precision. The field of photochemistry utilizes spectroscopy extensively. The existence and nature of molecular fragments which cannot be isolated chemically but which are important links in a chain of steps making up photochemical reactions have been demonstrated spectroscopically. As an example: OH radical, (Di-atomic hydroxides) – its properties such as inter-atomic distances, vibration and rotation frequencies, electronic states, etc., have been determined by spectroscopic methods in minute detail.

Spectroscopy in Physics

The spectroscopic data gives the most precise standards of length. It has suggested the standard of length as wavelength of a sharp red line emitted by cadmium atoms (6438.4696 Au) or sharp green line emitted by mercury atom of isotopes 198 (5460.740 Au). These wavelengths are more constant over long periods than that of man made standard (metre).

Electronic structures of atoms, magnetic susceptibility, etc., can be determined by spectroscopic means – Zeeman effect and hyperfine structure. The spectroscopy gives rise to different excitation spectra of an atom when electrons are being removed gradually one by one from an atom. Removal of an electron from an atom results in new set of spectral lines of the same atom. The study of the same informs about the energy levels and state of ionization of the atom.

Spectroscopy in Astronomy

The spectroscopy has given rise to vital informations regarding the constitution of heavenly bodies both qualitatively and quantitatively. The constitution of the surface of the Sun and the way in which it gives rise to energy, etc., are known to the scientists by the spectroscopic observation only. Spectroscope has identified about sixty-six elements in Sun, stars, and most distant nebulae. Doppler effect of spectral lines of stars is useful in measurement of approach and recession velocities of stars.

Spectroscopy in Biology and Medicine

Metallic elements in Biochemical substances, cells and tissues can be determined qualitatively and quantitatively by emission Spectroscopic methods. This helps the Biologists to determine various trace elements needed by cells for life and its growth.

In medical field, the spectroscopy is a useful tool to determine accumulation of lead, copper etc., in blood and tissues of people exposed to such materials in daily work.

Study of complicated molecular structures of vitamins, enzymes

co-enzymes are made simple by ultraviolet spectrophotometer and Raman Spectroscopy.

Spectroscopy in Food Research

Testing and controlling the production of foods and its containers are being taken up with spectroscopic methods. Condensed milk, chocolate products, tinned food industry, etc., find the spectroscopic methods indispensable as the methods can identify the elements (lead, copper, etc.) even in parts per million (ppm) level. Florescence spectroscopy is useful in testing liquid food, liquors and vitamin contents in it.

Spectroscopy in Metallurgy and Mineralogy

Speed and accuracy of spectroscopic methods make it a valuable tool in metallurgical industries. The sample it needs is very less so that it is called 'Non-destructive test'. Smelting and arcing process can be controlled due to the speed of analysis of specimen samples in Steel industry, Copper industry and Aluminum industry. Alloy plants make use of spectroscopic method as inevitable tool to control the addition of alloying materials.

Florescence spectroscopy plays a very important role in identifying the minerals.

Spectroscopy in Forensic Science

Highly established forensic laboratories make use of spectrography as a tool in crime investigation. The minute amount of stain on glass jar, dust in old trousers, paint sample of a car due to hit and run case, blood stains on a knife, pellet of shot removed from a person, broken pieces of a burglar's tool – may be analyzed spectroscopically to assist the detection of crime. The main advantage of this method is that, the analysis can be done accurately with the available small amount of samples.

Conclusion

This attempt to analyze the use of spectroscopic measurements in different fields of science is only to introduce it to laymen. Hence, many technical details have been screened so as to make it more general.

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