

Spectroscopy –An Analysis

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Abstract— Spectroscopic investigations have proved vital in our knowledge of the structure of atoms and molecules. Atomic spectra given us information about the arrangement and motion of electrons in an atom have led to the discovery of electron spin and understanding of periodic classification of elements. Molecular spectra provide information regarding the molecular binding motion of nuclear and electrons in the molecule and the structure of molecules. This information has played a great role in the development of quantum mechanics which in turn has provided a sound basis for the understanding of atomic and molecular spectra and structure. In spectroscopic observations, we need three kinds of devices i.e. light sources, spectrometers and detectors. Spectroscopy deals with interaction of electromagnetic radiation with matter and is the most important tool for investigation structure of atoms and molecules. Atomic vapor of alkalis give absorption spectrum of hydrogen atom. Some applications of atomic spectra as: important role in understanding the structure of atoms and their properties; development of modern atomic physics is due to the success of atomic spectra, atomic spectroscopy is a powerful analytical tool for ores and minerals. Some application of molecular spectra as: pollutants present in traces can be monitored and identified, crystal structures of crystals containing complex ions like SO_4 , NO_3 , CO_3 etc. structural information of high temperature superconductors have been obtained.

Key words: Spectroscopy, Emission and Absorption Spectra, Atomic Spectra

I. INTRODUCTION

Spectroscopy deals with interaction of electromagnetic radiation with matter and is the most important tool for investigating structure of atoms and molecules. Studies of atomic spectra have given us information about the arrangement and motion of electrons in an atom has led to the discovery of electron spin and understanding of periodic classification of elements. Molecular spectra provide information regarding the molecular binding motion of nuclear and electrons in the molecule and the structure of molecules. This information has played a great role in development of quantum mechanics which in turn has provided a sound basis for the understanding of atomic and molecular spectra and structure.

In spectroscopic observations we need three kinds of devices-

A. Light Sources

There are needed to produce light for spectroscopic investigations these may be classified in to temperature radiations and all kind of luminescence includes all forms of light emission in which kinetic heat energy is not necessary required in the excitation mechanism electrical discharge from sparks arcs or heissler tubes of different kinds operating on direct or alternating currents of direct or alternating currents of low or high frequency give emission

called electroluminescence. Fluorescence results from, excitation by absorption of light.

B. Spectrometers

Three types of spectrometers are now-a- days in use for repatriating wavelength component of emission or absorption spectra. These are based on refraction, diffraction and interference of light, principal of refraction is used in prism spectrometers and that of diffraction is employed in grating spectrometers. Their dependence on wavelength is in opposite sense, higher the wavelength lower is the refraction but diffraction is higher. The spectrometers based on interference principle are furrier-transform spectrometers. These are the latest fully computerized and most effective.

C. Detectors

A large number of Photo-detectors are nowadays employed depending upon their response, sensitivity and efficiency in different spectral regions for visible and ultraviolet regions the oldest in use are photographic plates or files. Among the modern ones are photo-electric or photomultipliers photo-emissive diodes, ccd detectors etc.

II. EMISSION AND ABSORPTION SPECTRA

Source of light we can excite the characteristic spectra of any substance. If the process involves absorption of energy by the material to excite it to a higher energy state, then after de-excitation the matter emits the some energy. This exited energy when passed through a spectrometer an emission spectrum is produced. This spectrum is characteristic of the substance. This is also called as spontaneous emission. There is another type of emission known as induced emission. This occurs when a substance is placed in its excited state in a field of radiation of energy matching with energy of excitation has the some energy as the inducing field and moves in same direction this gives a coherent radiation the incident beam is absorbed at the characteristic wavelength of the substance which goes to excited states and energy of the incident beam at remaining wave light moves forward. When the substance returns back to its ground state, it emits the absorbed energy. This is called absorption spectrum.

III. TRANSMISSION PROBABILITIES AND SELECTION

In spectroscopy, bohr atom model assumption is that an emission or absorption of radiation takes place due to electronic jump from one stationary orbit to the other no explanation could be provided for the relative intensities of different lines in atomic spectra This problem was taken care of by quantum mechanics from evaluation of transition probabilities and selection rules between different states of the action. When electron excited to an upper state of the atom stays there for some time before making a transition to its lower state. The time taken in a transition is inversely proportional to the transition probability for this transition.

The mean life time of an excited state is of the order of 10.8 s. The intensity of emission or absorption of radiation by a large number of atoms is proportional to the magnitude of the transition probability for the given transition.

Frequency of the bohr Atom

$$V = \frac{E_n - E_m}{h}$$

Using the expressions of the wave functions and carrying out their detailed calculation we get non-zero bohr atom model assumption that no values for there for change of n by any value and that for the angular quantum number.

$$\Delta l = \pm 1$$

These are called selection rules for atomic spectra.

IV. ATOMIC SPECTRA OF HYDROGEN ATOM

The interaction of electromagnetic radiation with matter and is the most important tool for investigating structure of atom and molecules. White light is dispersed by a prism into its constituent colors which he called a spectrum.

Formulas for hydrogen series

$$V_n = \frac{R}{n_1^2} - \frac{R}{n_2^2}$$

Here R is rydberg constant and n_1, n_2 integral number.

For laymen series

$$V_n = \frac{R}{1^2} - \frac{R}{n^2}$$

Balmer series

$$V_n = R \left(\frac{1}{2^2} - \frac{1}{n^2} \right) \text{ where } n=3, 4, 5, \dots$$

Paschen series

$$V_n = R \left(\frac{1}{3^2} - \frac{1}{n^2} \right) \text{ where } n=4, 5, 6, \dots$$

Brackett series

$$V_n = R \left(\frac{1}{4^2} - \frac{1}{n^2} \right) \text{ where } n=5, 6, 7, \dots$$

Pfund series

$$V_n = R \left(\frac{1}{5^2} - \frac{1}{n^2} \right) \text{ where } n=6, 7, 8, \dots$$

Knowing the value of R from the well-known balmer series the wave numbers of the lines of other series can be predicted with considerably accuracy.

V. MAGNETIC MOMENT OF THE ATOM

The ratio of the magnetic moment associated with the orbital motion of an electron to its mechanical moment known as gyro magnetic ratio, can be given as

$$\frac{\mu}{P} = \frac{e}{2mc}$$

$$\mu = \frac{eh}{4\pi mc}$$

Thus the magnetic moment of hydrogen atom should always be equal to an integral number of units

$$\frac{eh}{4\pi mc} \text{ ampere m}^2$$

This unit is called Bohr magneton.

VI. ELECTRONIC SPECTRA

Potential function of a diatomic molecule governing the motion of its nuclei. Considering for a moment the electronic

motion in a molecule for a fixed nuclear configuration, it is clear that the electronic energy will depend on the inter nuclear separation r. this dependence will be different for different electronic states. Since the electrons are much lighter than the nuclei, the electrons move much faster than the nuclei. Therefore, when the nuclei move the electronic energy takes up the value corresponding to the momentary positions of the nuclei. Thus in changing the nuclear positions work is done against the coulomb repulsion of the nuclei and also to change the electronic energy. In other words the sum of electronic energy and coulomb repulsion energy provides the potential energy. Which governs the nuclear vibrations in a molecule? Usually the minimum of the potential energy function of a given stable electronic state is considered as the electronic energy of the state.

Total energy E_{tot} of the molecule is written as

$$E_{tot} = E_{elac} + E_{vib} + E_{rot}$$

In wave number it is written as

$$T = T_{elo} + G(V) + F(J)$$

VII. CONCLUSION

With the development of most sensitive spectrometers and power laser excitation sources as well as newer detection techniques. Some of the important applications in structure determination and identification of material is like structural information can be obtained only by the study of raman spectra. In highly symmetrical polyatomic molecules infrared and raman spectra are complimentary to each other so study for both necessary raman spectroscopies has also been used in the study of chemical bonds in biological samples. Structural information of high temperature super conductor have been obtained by spectroscopy pollution also traces with the help of spectroscopy.

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