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MODERN RESEARCH METHODS AND APPLICATION OF PHYSICAL SCIENCES

Begmuradov Shokhzod Dilmurodovich
Jizzakh State Pedagogical University
Student of the Faculty of Physics and Astronomy

ABSTRACT

This article discusses modern research methods and their use in physical science.

Keywords: Modern, research methods, NMR, correct function, inverse function, physical properties of the molecule.

One of the main issues of chemistry is the definition of what a substance is and its structure. This work used to be solved by chemical methods, but now it is solved mainly by physical methods. Usually, a chemist begins the study of a substance by determining which elements the lmi consists of, and finds the gross formula. Only after that he tries to determine the structure of his molecule.

If the chemical process is being studied, then the question also arises of determining the components of the mixture formed as a result of the reaction at a certain stage of this process, as well as the quantitative characteristics of the compound. From a methodological point of view, the study of the physical properties of a substance and a molecule, as a science, is connected with the studied substance and the physical field acting on it (electric, magnetic, electromagnetic...) the type of incoming frequencies "numbers" (X-ray, ultraviolet, visible, infrared, radio waves..) or a special section of the theory that studies the interaction of particles with a rod (electron, neutron). As a result of such an impact, certain properties of the substance and its molecules manifest themselves.

The immediate task of the physical method is to determine the changes in the light incident on the substance, the beam of particles and various physical fields acting on it after their interaction with the substance. Studying the interaction of electromagnetic rays, particles and physical fields of each frequency with matter, i.e., according to the results of the experiment, determining the physical properties of matter and finding the physical quantities of the molecule is part of the solution of the problem from the reverse side and is called the inverse problem of the physical method.

For example, when analyzing nuclear magnetic resonance (NMR) spectra with high resolution, it is not difficult to distinguish between the correct and inverse problems of this method. The correct function. Taking into account the value of chemical shifts and spin-spin interaction constants of the corresponding substance, it is required to calculate its NMR spectrum. The inverse function. The substance is given by the NMR spectrum obtained in the experiment, from which it is required to determine the chemical shifts of the corresponding nucleus and the spin-spin effect constants. As a rule, the solution of the inverse problem is of practical importance.

Currently, spectroscopic methods are widely used in chemistry within the framework of physical research methods. Using these methods, the dependence of the intensity of electromagnetic rays emitted or absorbed by a substance on the frequency or wavelength of their NMH is studied.

Spectroscopic methods to find the difference between the electronic, vibrational, rotational and magnetic energy levels of atoms and molecules, energy levels through the intensity of the spectral band. Studying them, in turn, makes it possible to find the symmetry of the molecule, the geometry of which atoms it consists of, electrical properties and other quantities.

The frequency, intensity, width and shape of the spectral band are related to the properties of the substance, many sizes of the molecule. Spectral analysis of these problems the methods can be investigated by solving the inverse problem. The use of physical methods makes it possible to investigate the main issues of the theory of chemical structure. These include: ketrna sequence and multiplicity of chemical bonds, optical and conformational isomerism, interatomic coordination number, interaction of atoms and atomic groups in molecules, internal rotations in the molecule and other types of motion with a large amplitude, energy, electrical and other characteristics of molecules, intermediates formed as a result of the reaction, and reaction mechanisms etc.

In general, quantitative data, which will become the basis of modern quantum and theoretical chemistry, are mainly obtained using physical research methods. Among the physical research methods most commonly used for solving chemical problems include: nuclear magnetic resonance spectroscopy (NMR), infrared light absorption spectroscopy (IR), mass spectrometry and electron absorption spectroscopy. The process of obtaining knowledge in physics and chemistry is carried out by observing physical and chemical phenomena in natural conditions or by conducting special experiments. Experience in general is an important part of the learning process.

Depending on the wavelength range of electromagnetic radiation used and the nature of the corresponding transitions, atomic spectroscopy methods are divided into optical and X-ray spectroscopy. The methods of optical spectroscopy use ultraviolet and visible regions of electromagnetic radiation. It corresponds to a change in the energy of valence electrons. To obtain atomic-optical spectra, it is necessary to spray the sample beforehand, that is, to transfer it to a gaseous atomic state. This work can be carried out through atomizers, that is, high-temperature sources with different structures.

Depending on the physical nature of the interaction of electromagnetic rays with matter, atomic spectroscopy methods are divided into radiation and absorption methods. In optical radiation methods, atoms must be converted to an excited state in order to obtain a spectrum of radiated rays.

Emission optics methods in which atoms are excited and exposed to high temperatures are called atomic emission spectroscopy methods. These methods use a single device, an excitation source, to convert matter into atoms and excite bonds.

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Spectroscopy, including molecular spectroscopy, is a science that studies the structure and properties of molecules that make up a substance through the processes of absorption, return and scattering of electromagnetic waves in a substance. Various substances in different aggregate states can be used as an object of spectroscopic studies. The simplest case of such objects

these are rarefied gases whose molecules are located at a distance from each other, which allows them to be considered independent. However, the most difficult case is a condensed medium, each particle of which participates in intermolecular interaction. Spectroscopic data can provide information not only about the structure and properties of the molecule, but also about the forces of interaction between molecules, as well as about the structure of matter. As you know, the distribution of electromagnetic radiation energy along the wavelength is called the spectrum. Depending on the interaction of radiation with matter, the radiation spectrum, the absorption spectrum, the scattering spectrum and the return spectrum are distinguished. Spectroscopy as a whole is studied, divided into atomic-nuclear spectroscopy, molecular spectroscopy and crystal spectroscopy.

Each region provides information about a specific type of motion of the molecular system. For example, if information is obtained about electronic transitions in the field of view and ultraviolet, then in the infrared field it is possible to obtain information about the vibrations of the atoms of the molecule Around the equilibrium state.

The spectrum of the molecule gives complete information about the properties of the substance. Depending on the spectrum of the molecule, it is possible to obtain information not only about which molecules the substance consists of, but even about the mutual arrangement of atoms in the molecule, the isomers of the molecules.

First of all, it should be noted that, although the name of this phenomenon has the word "core", nuclear physics has nothing to do with IMR and has nothing to do with radioactivity. If we talk about a strict description, then we cannot do without the laws of quantum mechanics. According to these laws, the energy of interaction of a magnetic core with an external magnetic field can take several discrete values. If magnetic nuclei are radiated by an alternating magnetic field, the frequency of which is expressed in frequency units corresponding to the difference between these discrete energy levels, then magnetic nuclei begin to move from one level to another, absorbing energy.

Variable area... This is a magnetic resonance phenomenon. This explanation is formally correct, but not entirely accurate. There is another explanation without quantum mechanics. A magnetic core can be represented as an electrically charged ball rotating around its axis (although, strictly speaking, this is not the case). According to the laws of electrodynamics, the rotation of the charge leads to the appearance of a magnetic field, that is, the magnetic moment

of the nucleus directed along the axis of rotation. If this magnetic moment is placed in a constant external field, then the vector of this moment will begin to move forward, that is, rotate in the direction of the external field.

In the same way, the axis of rotation rotates (rotates) around the vertical, if it rotates at a certain angle, and not strictly vertically, gravity plays the role of the magnetic field in this.

The precession frequency is determined by both the properties of the core and the intensity of the magnetic field: the stronger the field, the higher the frequency. Then, if, in addition to a constant external magnetic field, an alternating magnetic field acts on the core, then the core begins to interact with this field - as if shaking the core harder, the precession amplitude increases, and the core absorbs the energy of the alternating field.

However, this happens only under conditions of resonance, that is, the coincidence of the precession frequency and the frequency of the external alternating field. It's like a classic example from high school physics - soldiers crossing a bridge.

If the step frequency coincides with the natural frequency of the bridge, then the bridge will vibrate more and more. Experimentally, this phenomenon manifests itself in the dependence of the absorption of an alternating field on its frequency.

One of these interactions is called a chemical shift. Its essence is as follows: the electron shell of the molecule reacts to an external magnetic field and tries to shield it - partial shielding by a magnetic field occurs in all diamagnetic substances. This means that the magnetic field in the molecule differs very little from the external magnetic field, which is called a chemical shift.

However, in different parts of the molecule, the properties of the electron shell are different, as is the chemical shift. Accordingly, the resonance conditions of the nuclei in different parts of the molecule will also be different. This makes it possible to distinguish chemically unequal nuclei in the spectrum.

it can be observed in different nuclei, but it should be said that not all nuclei have a magnetic moment. It often happens that some isotopes have a magnetic moment, while other nuclear isotopes do not.

In total, there are more than a hundred different isotopes of chemical elements with magnetic nuclei, but more than 1520 magnetic nuclei are usually used in research, everything else is exotic.

Each core has its own magnetic field characteristic and rotation frequency, called the gyromagnetic ratio. For all kernels, these relations are known.

With their help, it is possible to select the frequency at which the signal from the nuclei necessary for the researcher for this magnetic field will be observed. The most important nuclei for YMR are protons.

One of the most important and expensive parts of a spectrometer is a magnet that creates a permanent magnetic field. The stronger the field, the higher the sensitivity and resolution of the spectrum, so scientists and engineers always strive to get as many fields as possible. The magnetic field is created by an electric current in the solenoid - the stronger the current, the larger the field.

However, the current cannot be increased indefinitely; if the current is too high, the electromagnetic wire simply begins to melt. That is why for a very long time superconducting magnets have been used for high-field spectrometers, that is, magnets in which the

electromagnetic wire is in a superconducting state. In this case, the electrical resistance of the wire will be zero, and energy will not be released at any current value.
The conducting state can only be obtained at very low temperatures, only a few degrees Kelvin, which is the temperature of liquid helium.

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