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THE ROLE OF MATHEMATICS IN CHEMISTRY

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ABSTRACT

this article highlights the importance of mathematics in teaching chemistry. Also, in solving chemical problems, various methods using mathematical formulas are shown.

Science is developing rapidly modern education for young people everyone knows the urgency of the issue. Especially mathematical modeling and information community by creating technology programs and solving problems related to nature is mathematics. What is the importance of science in education shows ownership? Including in higher education mathematician of chemistry students if we talk about the limit of knowledge, Mathematics for chemists, first of all, many useful tool in solving chemical problems is considered Mathematics in chemistry in general. It is very difficult to find any area that is not used difficult. Functional analysis and group theory quant widely used in chemistry, probability theory is the basis of statistical thermodynamics, graphs theory of complex organic in organic chemistry in predicting the properties of molecules, differential equations are fundamental to chemical kinetics tool, topology in chemical thermodynamics and differential geometry methods are used. The term "mathematical chemistry" is in the lexicon of chemists firmly established. In serious chemical journals Many articles contain a single chemical formula if not, but with mathematical equations is filled [1].

For students of chemistry education to the program and curriculum of mathematics it is taught for two semesters. Science this year in the program of higher mathematics - analytic geometry and 7 lectures on elements of linear algebra, 18 lectures on the elements of mathematical analysis, 2 lectures on differential equations, probabilities 3 from the elements of theory

and mathematical statistics a lecture was given [2].

Mathematics for chemists is, first of all, a useful tool for solving many chemical problems. It is very difficult to find any branch of mathematics that is not used at all in chemistry. Functional analysis and group theory are widely used in quantum chemistry, probability theory is the basis of statistical thermodynamics, graph theory is used in organic chemistry to predict the properties of complex organic molecules, differential equations are the main tool of chemical kinetics, topology and differential geometry methods are used in chemical thermodynamics. The expression "mathematical chemistry" has firmly entered the lexicon of chemists. Many articles in serious chemical journals do not contain a single chemical formula, but are replete with mathematical equations .

It was mathematics that transformed chemistry from a descriptive science into an experimental one, and it was mathematics that made chemistry a science. It is with the help of mathematics that we make both the simplest calculations using chemical formulas and equations of chemical reactions, and the most complex mathematical operations that model the most complex chemical processes in both living and inanimate nature. No chemical production is possible without mathematics.

Chemistry does not have its own laws (the law of conservation of mass is a consequence of the general law of conservation of energy, and the periodic law obeys the rules of physics). Three theories of chemistry (quantum chemistry, chemical thermodynamics and chemical kinetics) form a special branch of science called physical chemistry.

Chemistry, instead of its own laws and theories, has a colossal variety of objects under study: about 60 million individual substances alone have been characterized in chemistry (not counting numerous mixtures). But there are also chemical reactions between substances. Only a very small proportion of substances known to chemistry (only a few percent) are found in nature, the rest of the substances are products of human activity. The outstanding American chemist Roald Hoffman believes that chemists differ from other scientists in that they create objects with their own hands, which they then perceive and study.

Chemists have a characteristic only for them, a unique view of the world around them, they "feel the substance." Modern chemists and physicists are able to work even with individual atoms and molecules. The primary tasks of chemistry are the search for new substances with useful properties, catalysts, medicines, building materials, energy accumulators.

With the help of mathematics, we make both the simplest calculations using chemical formulas and equations of chemical reactions, as well as the most complex mathematical operations that model the most complex chemical processes in both living and inanimate nature. No chemical production is possible without mathematics. If you imagine for a moment what would happen if numbers and mathematical calculations disappeared from chemistry. The world would be deprived of food, medicines, paints, photographic films, mineral fertilizers, plastics, metal alloys and many other useful substances and things. Mathematics for chemists is, first of all, a useful tool for solving many chemical problems. It is very

difficult to find any branch of mathematics that is not used at all in chemistry.

Functional analysis and group theory are widely used in quantum chemistry, probability theory is the basis of statistical thermodynamics, graph theory is used in organic chemistry to predict the properties of complex organic molecules, differential equations are the main tool of chemical kinetics, methods of topology and differential geometry are applied in chemical thermodynamics.

Let us dwell in more detail on the application of mathematics in chemistry. Mathematical equations and methods used in chemistry deal with specific properties of atoms and molecules. Therefore, mathematical equations used in chemistry, as well as their solutions, must have a chemical meaning. The role of mathematics in chemistry is great (many mathematical laws and formulas are used to solve chemical problems, but at the same time, chemistry imposes restrictions on the solution of mathematical equations, since they must have a chemical meaning) [3].

Higher education taught in foreign countries analysis of literature on mathematics it shows that they have an educational direction in teaching attention to education based on the characteristics is focused. These are practical skills of students has a positive effect on development. Mathematical problems with chemical composition solving the studied formulas to students and demonstrate the practical importance of theorems. Visualize the interaction of mathematics and chemistry students of the chemistry department motivation and level of mathematical culture allows to increase [4].

Applications of mathematics in chemistry are extensive and varied. We want to show one of the examples: the rate of a chemical reaction is a change in the amount of a substance per unit of time: for homogeneous processes - per unit volume, for heterogeneous processes - per unit interface. The mathematical notation of this definition can be written: in the form

or

where N - the amount of substance; t - is time; V - the volume; s - the phase separation surface [5].

As an example of typical tasks of computer chemistry, we can mention the study of various properties of complex molecules using the methods of forming hypotheses "structure-property" of chemical compounds that have not yet been synthesized, based on the methods of mathematical logic. These methods include methods of interval analysis, singled out as an independent area of applied mathematics and allowing one to take into account the conformational flexibility of molecules and obtain both qualitative and quantitative predictions of the properties of interest to the researcher.

One more example mathematical formulas are used to study the composition of complex compounds. Optimized Values of Energy Parameters of Calculated Molecules [6].

Interval analysis is a theory designed to take into account rounding errors when performing calculations on digital computers. Since the result of each rather complicated calculation contains some error due to rounding errors of the input data and intermediate results, to take into account this error, each value can be represented by a pair of numbers that limit

it from below and above and have an exact representation in the computer.

Thus, each value is replaced by a certain number containing with an interval. When doing arithmetic actions, the new interval is calculated using special operations. The method of complex interval models is based on the use of interval estimates of the quantum chemical parameters of organic compounds. Using interval methods makes it possible to identify and analyze ambiguous "structure–activity" dependencies. The method was used in the computer solution of the problems of predicting the anti-tuberculosis activity of dithiocarbamic acid derivatives; maximum absorption of chlorophyll derivatives, which made it possible to select the most promising basic structures of drugs for photodynamic cancer therapy from a group of compounds.

Computational chemistry should not be confused with computational chemistry. Computational chemistry is a branch of chemistry that uses computers to solve chemical problems. Computational chemistry uses the results of classical and quantum theoretical chemistry, implemented in the form of efficient computer programs, to calculate the properties and determine the structure of molecular systems. In quantum chemistry, computer simulations have replaced not only traditional analytical calculation methods, but in many cases complex experimentation as well. Computational chemistry makes it possible in some cases to predict previously unobserved chemical phenomena.

Computational chemistry is actually a new way of conducting scientific research in chemistry - computer experiment and computer simulation. Traditionally, experimenters conduct chemical experiments with real chemical systems, and then theorists explain the results of these experiments in terms of developed models and theories.

This approach has been successful until recently, and now we know the basic laws that describe chemical phenomena and processes. However, their exact analytical description is often possible only in the case of very simple models. Approximate analytical methods make it possible to expand the set of problems to be solved. The development of computers over the past 60 years has made it possible to solve many problems not only in the case of simplified models, but also for real chemical processes and structures [6-7].

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