CHEMICAL SCIENCES

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USING THE VECTOR APPROACH FOR PROBLEMS OF CHEMICAL STOCHIOMETRY

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Abstract: The basic principles of using a vector approach for solving problems of chemical stoichiometry are presented. Examples of using the method for various chemical systems are given. It is shown that the use of a vector approach for solving problems of chemical stoichiometry provides a powerful tool for the study of complex chemical systems, allows you to visually display the interactions between various reagents and graphically display, show, notice different types of chemical reactions, quickly find stoichiometric coefficients for chemical equations without using mathematical methods any type and quantity of reagents, allows to develop new mathematical methods of balancing reactions.

Keywords: chemical reactions, systems of equations, stoichiometric coefficients, vectors, algorithm, graphic analysis.

Balancing chemical reactions is one of the most important and mandatory parts of modern chemistry. Methods of balancing reactions are taught from the first chemistry lessons, but for most students they remain unclear [1-2].

The situation becomes even more complicated when working not with individual chemical equations, but with systems of equations, electrochemical half-equations, and transformations of organic compounds [3].

One of the main reasons for this is the use of purely mathematical methods and various mnemonic rules, that is, the absence of a visual connection with chemical objects.

The use of a vector approach to this problem makes it possible to establish such a connection due to the graphic display of interactions between parts of chemical systems [4-6].

Each part of a chemical system (molecule, ion, radical, formula unit) can be represented in the form of a multidimensional vector with integer values for each of the elements (hereinafter compound).

$$H_2SO_4, NaOH$$

$$H_2S_1O_4, Na_1O_1H_1 \rightarrow \vec{c} = \{e_H, e_S, e_O, e_{Na}\} \rightarrow \vec{c}_{H_2SO_4} = \{2,1,4,0\}, \vec{c}_{NaOH} = \{1,0,1,1\}$$

The total number of elements in a chemical system is the sum of all elements of all compounds

$$H_2SO_4 + 2NaOH \rightarrow H_4S_1O_6Na_2$$

Addition to the system of compounds affects only the number of elements that are present in this compound, so we can speak of the independence of the number of elements from each other and from the set of compounds.

Thus, the sum of vectors with a limited set of elements can be considered separately, which corresponds to the projection on the selected axes of the multidimensional space.

As an example, we can cite the reduction of dimension for reactions with

$NH_3+2O_2=HNO_3+H_2O$ - full reaction in space $\{e_N,e_H,e_O\}$

$N+2O_2=NO_3+O$ - projection on $\{e_N,e_O\}$

$H_3+2O_2=HO_3+H_2O$ - projection on $\{e_H,e_O\}$

$NH_3=HN+H_2$ - projection on $\{e_N,e_H\}$

$N=N$ - projection on $\{e_N\}$

$2O_2=O_3+O$ - projection on $\{e_O\}$

$H_3=H+H_2$ - projection on $\{e_H\}$

This fact is very important, because it allows you to visually display the composition of chemical systems and leads to a number of solutions with them.

The first and very important consequence of using the vector approach is the formulation of the reaction mixture as a point in a multidimensional space, the location of which is determined by the sum of compound vectors, which can be defined as base vectors. In essence, such a point is the total composition of a mixture of all compounds.

Since the base vectors have integer and positive values for each of the coordinates, not all points in space can be represented by the sum of the base vectors, and some can be represented by more than one combination of vectors.

In the first case, it corresponds to a simple mixture of compounds, in the second case, it corresponds to a chemical reaction.

That is, from the point of view of the vector approach, the reaction is the presence of two or more sums (combinations) of compound vectors that have a common end point in the multi-element space, and the number of such vectors corresponds to the stoichiometric coefficients of the chemical equation.

It should be noted that this approach slightly expands the concept of a chemical reaction due to the possibility of the existence of the same compound in both parts of the equation, as well as the possibility of forming multiple values of the coefficients (Fig. 1).

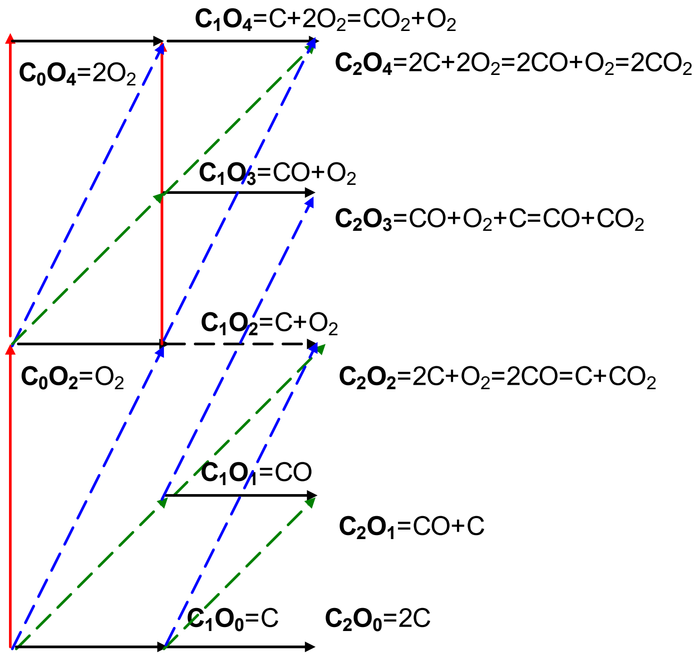

Fig. 1. Scheme of chemical reactions in a two-element vector space

When reducing the compounds in the equation and reducing the values of the coefficients to the lowest multiple, we obtain classical chemical equations for each point of the multidimensional elemental space

1. $C_0O_{2n} \rightarrow O_2$ - a mixture of molecules O_2
2. $C_0O_{2n+1} \rightarrow$ does not exist for this set of compound vectors
3. $C_0C_n \rightarrow$ C - a mixture of atoms C
4. $C_1O_1 \rightarrow$ - only in form CO, has no other combinations of vectors
5. $C_1O_2 \rightarrow C+O_2$ and compound CO_2 - chemical reaction $C+O_2 = CO_2$
6. $C_1O_3 \rightarrow$ - a mixture of individual compounds CO та O_2
7. $C_1O_4 \rightarrow$ - combinations $C+O_2+O_2$ та CO_2+O_2 - can be reduced to the reaction $C+O_2 = CO_2$
8. $C_2O_1 \rightarrow$ a mixture of individual compounds CO та C
9. $C_2O_2 \rightarrow$ combinations CO, $C+C+CO_2$ та $C+CO_2$ - chemical reactions $2CO = C+CO_2= 2C+O_2$
10. $C_2O_3 \rightarrow$ combinations $C+CO+O_2$ та $CO+CO_2$ - can be shortened to $C+O_2 = CO_2$ 1
11. $C_2O_4 \rightarrow$ combinations $CO+CO+O_2$, $C+C+O_2+O_2$ та CO_2+CO_2 -

chemical reactions $2CO+O_2 = 2CO_2$ та $C+O_2=CO_2$

It should be noted that from the diagram in fig. 1 it is very clear that the classical chemical equation is not the same as the real chemical equation, since they can be of different nature, which must be taken into account when creating and studying large systems of chemical equations (CNR).

A classical chemical equation is only a part of a general set of chemical equations in which sets of reactants and products do not have common (identical) compounds and have minimal whole positive coefficients. The number of classical equations for each system is finite. Not every point in a system of chemical equations has a classical equation, but every point can be represented by a linear combination of classical chemical equations.

As you can see, for two points, three sets of compound vectors are possible at once, which can be reduced to only four classical chemical equations

$$2C+O_2 = 2CO \qquad \{1\}$$

$$C+O_2 = CO_2 \qquad \{2\}$$

$$C+CO_2 = 2CO \qquad \{3\}$$

$$2CO+O_2 = 2CO_2 \qquad \{4\}$$

According to them, the same composition can be obtained by two different combinations of compounds, which graphically reflects the concept of parallel reactions. Reactions {1}{3} and {2}{4} are parallel.

At the same time, reaction {4} can be obtained as the sum of reaction vectors {1} and vector O_2, and reaction {3} as the sum of reaction vectors {2} and vector C. This graphically corresponds to sequential reactions. Thus, reactions {1}{4} and {2}{3} are consecutive.

The use of the vector method for oxidation-reduction reactions allows you to visually display the degrees of oxidation of elements in compounds and allows you to find all possible chemical reactions between them (Fig. 2).

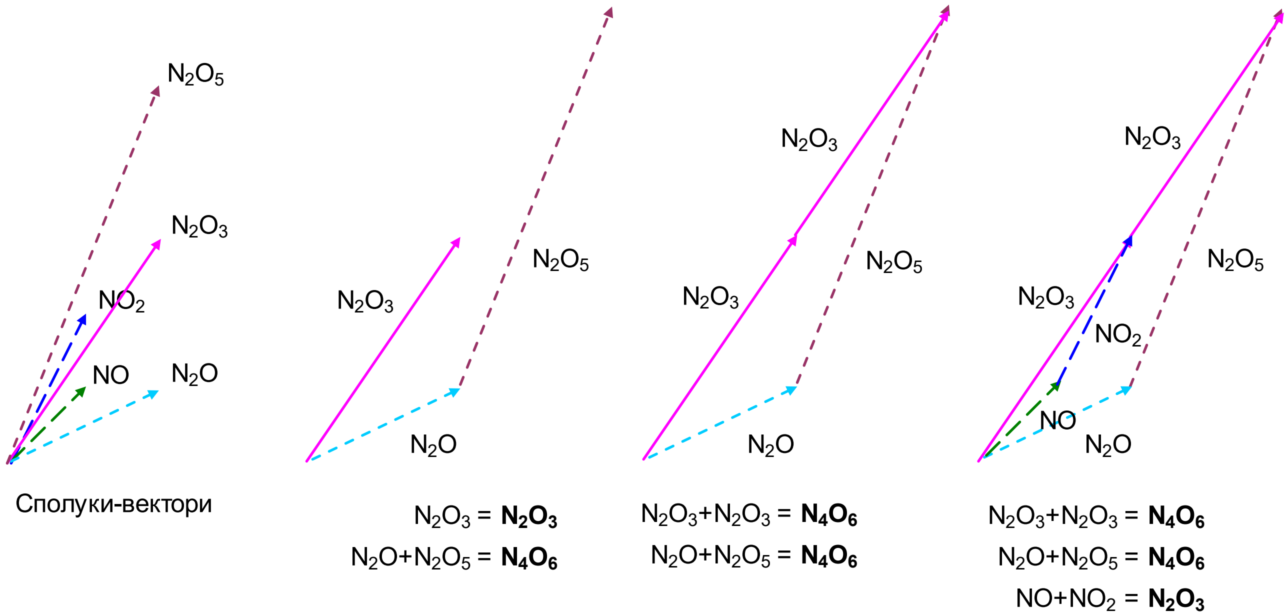

Fig. 2. The sequence of finding stoichiometric coefficients for reactions with a change in the degree of oxidation of elements

For reactions without a change in the degree of oxidation (combination or disintegration, neutralization), it gives only one possible reaction (Fig. 3).

But for exchange reactions, it is necessary to use not two-element vectors, three-element or consecutive sets for two different combinations of two-element vectors (Fig. 4).

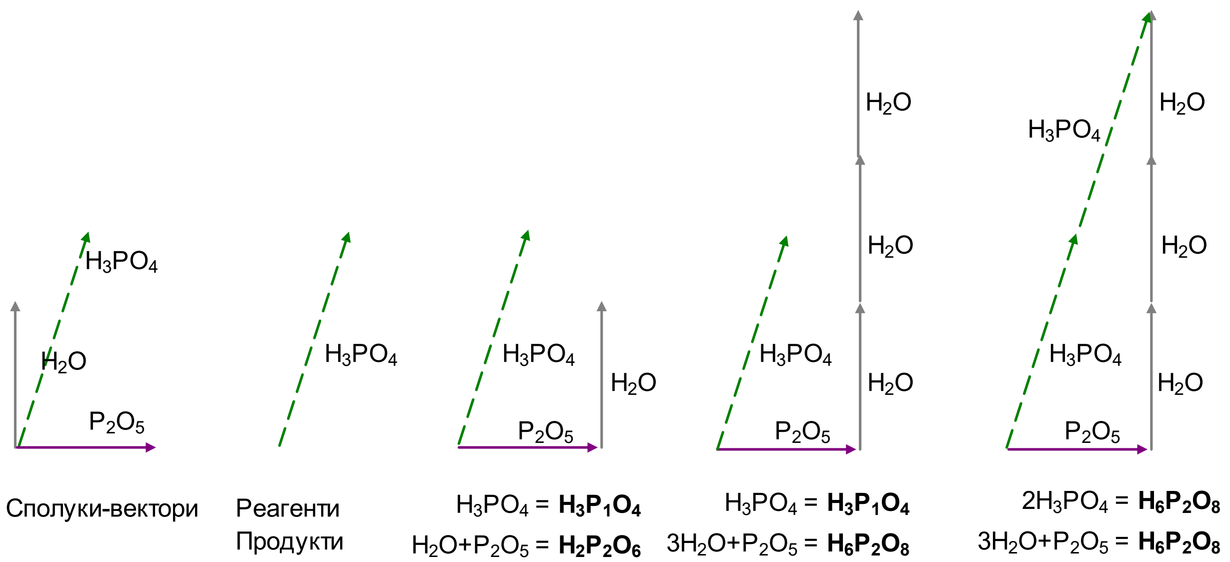

Fig. 3. The sequence of finding stoichiometric coefficients for reactions without changing the degree of oxidation of elements

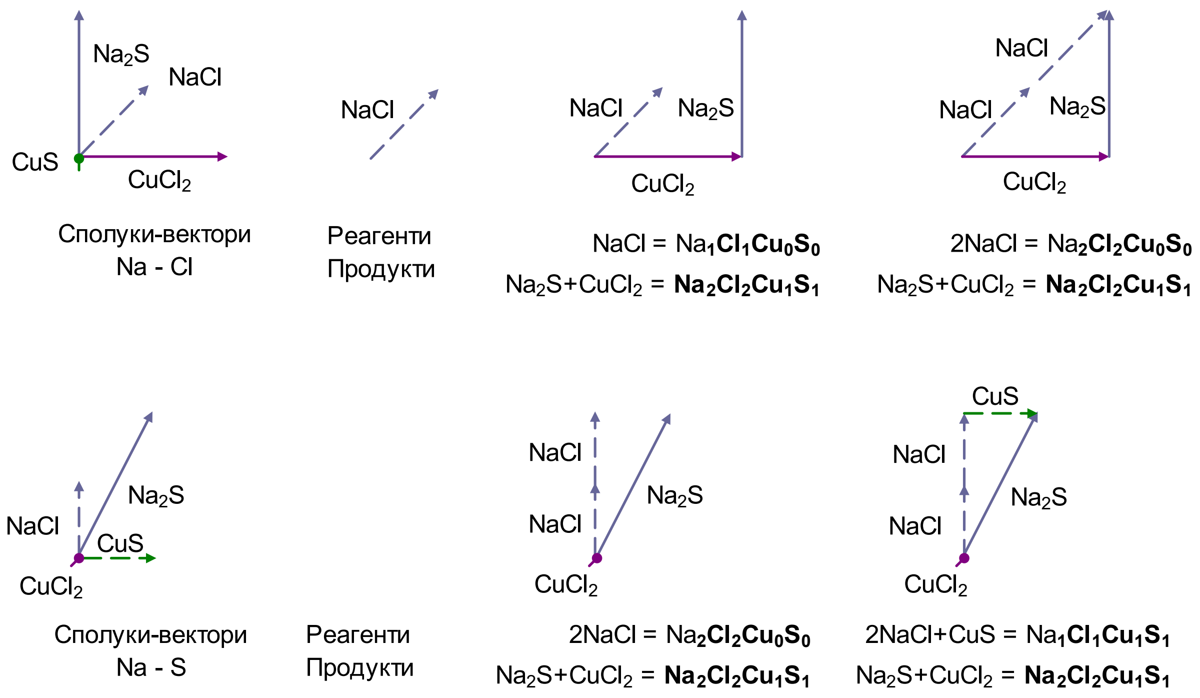

Fig. 4. The sequence of finding stoichiometric coefficients for exchange reactions

Thus, the use of a vector approach to solve problems of chemical stoichiometry provides a powerful tool for the study of complex chemical systems, allows you to visually display interactions between various reagents and graphically display, show, notice different types of chemical reactions, quickly find stoichiometric coefficients for chemical equations without using mathematical methods any type and quantity of reagents, allows to develop new mathematical methods of balancing reactions.

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