Kaplunenko Volodymyr G.
"Nanomaterials and Nanotechnologies Ltd",
Ukraine
e-mail: kaplunenkov@gmail.com

Kosinov Mykola V.
"Nanomaterials and Nanotechnologies Ltd",
Ukraine
e-mail: nkosinov@ukr.net

LAWS OF HETEROGENEOUS CATALYSIS

Abstract. *Based on the generalization of experimental and theoretical studies in the field of catalysis, three basic laws of heterogeneous catalysis were discovered. From the formula of the catalysis rate law, the most important characteristics of catalysis are obtained - the reaction output, TOF and TON. Formulas for calculating the characteristics of catalysis using the characteristics of catalyst substance are given. A new concept of heterogeneous catalysis has been developed, in which the role of catalysts in the mechanism of accelerating chemical reactions has been revised. The oxidation states of the reactants and active sites of the catalyst are used as parameters in the formulas of the laws of catalysis. It follows from the laws of catalysis that oxidation states are such important characteristics of catalyst substance and reagents, that they directly affect the mechanism of catalysis itself and set the values of the most important characteristics of catalysis. As the main tool in the selection of catalysts, it is necessary to use the list of oxidation states of chemical elements known in chemistry. Based on the laws of catalysis, new definitions of catalyst and catalysis are given. The class of catalysts is expanded. Material catalysts are complemented by field catalysts. The substantiation of catalysis as a fundamental direction in science is given.*

Keywords: *Laws of catalysis, electrons and protons in catalysis, catalysts - carriers and generators of electrons, calculation of TOF and TON, calculation of ROF and RON, field as a catalyst, donor-acceptor mechanism of catalysis, overcoming the Sabatier maximum, catalytic resonance, oxidation states.*

1. Introduction

Despite the almost 200-year history of catalysis, due to the complexity of catalytic reactions and their diversity, a theory of catalytic action has not yet been created that could predict the catalytic properties of substances and allow theoretical calculation of the rates of catalytic reactions. With a sufficiently large number of hypotheses, theories, principles and rules in the field of catalysis, his history shows that many of the fundamental discoveries in catalysis were made either by chance or empirically by enumeration of a large number of substances. There is no rigorous quantitative theory that could universally, using a single equation, describe the dependence of the rate of a catalytic reaction [1–3]. The mechanism of catalytic activation, which has not yet been revealed in the existing theories of catalysis, remains a big mystery. Naturally, such a way of developing the doctrine of catalysis does not correspond to the modern level of science.

The absence of a scientific theory of catalysis capable of predicting the catalytic properties of substances against the backdrop of an abundance of unsuccessful theoretical concepts and local theories of catalysis gave rise to disbelief in the possibility of creating a “good” theory of catalysis and gave rise to the assertion that «*catalysis is more of an art than a science»* which is repeatedly found in specialized literature [1, 4, 5].

The preparation of catalysts is also considered an art and recipes for their preparation must describe all operations in detail so that the preparation procedure is reproducible. A successful "recipe" is mostly created by trial and error, and not by scientific analysis of the processes occurring during the synthesis [4 - 6]. As noted in [6], «*this is more like a culinary art (l’art de cuisine) than a stoichiometric chemical synthesis».*

In publications one can come across the assertion that *«it is impossible in principle to explain such a complex phenomenon as catalysis within the framework of a unified theory»* [7]. The author of the chain theory of catalysis, N. N. Semenov, connected the creation of a general theory of catalysis with the solution of an even more complex problem in chemistry - the creation of a general theory of the reactivity of substances. He believed that the creation of a general theory of catalytic phenomena is possible *"not earlier than the creation of a general theory of reactivity"* [8].

Such uncertainty about scientific nature of catalysis and attempts to classify it as an art, to a large extent hinder the development of catalysis. In catalysis research, there is clearly a lack of new ideas that make it possible to consider the problems of the catalytic phenomenon from fundamentally new positions.

2. On the theories of catalysis

No other science has developed so many different theories to explain just one phenomenon, as happened in catalysis. At the same time, none of the developed theories of catalysis made it possible to discover the laws of catalysis, theoretically calculate the rates of catalytic reactions, or predict the catalytic properties of substances. An abundance of theories (Berzelius' theory of catalysis, D.I. Mendeleev's theory of bulk intermediates, Faraday and Schwab's adsorption theory of catalysis, P. Sabatier's theory of surface intermediates, H.S. Taylor's theory of active centers, A.A. Balandin's multiplet theory, theory active ensembles by N.I. Kobozev, the electronic theory of catalysis by D.A. Douden and F.F. Volkenshtein, the chain theory of catalysis by N.N. Semyonov and V.V. Voevodsky, the theory of supersaturation by S.Z. Roginsky, etc.) can point out that the development of a quantitative theory of catalysis is still too far away.

According to B.V. Romanovsky, the listed theories are not such stated - they are more theoretical concepts than theories. *«They are not general, but particular models that belong to a relatively narrow range of catalytic systems»* [1]. «They have a «local» character, as well as other less well-known theoretical concepts, and only qualitatively, although very convincingly, can explain a relatively small range of catalytic phenomena related to heterogeneous catalysis» [1].

A common shortcoming of all developed theories of catalysis is that they explained catalysis only qualitatively, not quantitatively. They do not define what type of interaction, out of the four fundamental interactions known in nature, is realized in catalysis. Within the framework of theories, the laws of catalysis and the requirements for the characteristics of the catalyst substance are not formulated.

This does not mean that the theories developed in catalysis were useless. Each of them has contributed to the science of catalysis. This is a great work of great scientists. Despite the local nature of the theories, they, albeit fragmentarily, but revealed the secrets of catalysis, each in its own local area of catalysis. What is missing now is the generalization of all theoretical concepts and the unification within the framework of one quantitative theory of catalysis of «good» fragments taken from previously developed theories.

3. Why are the laws of catalysis not discovered?

A paradoxical situation has developed in catalysis. Despite the abundance of theories of catalysis, none of them led to the discovery of the laws of catalysis. The main reason can be considered the absence of a quantitative theory of catalysis. Another reason is that faith in the possibility of creating a general theory of catalysis was lost, and catalysis was increasingly considered not a science, but an art [1, 4, 5]. Naturally, it is difficult to find a place for scientific laws in catalysis if catalysis is not considered a science. The laws of catalysis are sometimes called general principles and rules that have a phenomenological nature. For example, in specialized literature on catalysis, one can find following formulations: «Berzelius's law of catalysis», «Ostwald's law of catalysis», «Sabatier's law of catalysis», «Sabatier's principle», «Boreskov's rule» [9 - 12].

The Berzelius law of catalysis in [9] refers to the definition of a catalyst as a substance that enhances a chemical reaction, but itself remains unchanged as a result of the reaction.

Ostwald's law of catalysis in [9, 10] considers the definition of a catalyst from the point of view of chemical thermodynamics: the catalyst does not change the equilibrium between the reaction and product molecules, but increases or suppresses the rate of their reaction. As Rutger A. van Santen notes [9, 10], Ostwald's catalysis law does not provide a recipe for developing an optimal catalyst.

Sabatier's law of catalysis [9] states that in a catalytic reaction the reacting molecules form intermediate complexes with the catalyst. These complexes should have intermediate stability - neither too stable nor too unstable. The Sabatier principle, as it is more commonly called, also does not provide a recipe for determining the activity of a catalyst depending on its chemical structure. According to Rutger A. van Santen, «this formulation of the Sabatier law is more like an implicit invitation to formulate a theory of catalyst activity depending on the composition of the catalyst» [9, 10].

The above laws can hardly be called the laws of catalysis in the strict scientific sense. These are just the rules and principles of catalysis, which, like the Boreskov rule, have not been finalized to the level of scientific laws. To transform these rules and principles into laws of catalysis, a theory is needed in which these rules and principles will change from qualitative to quantitative and will be represented by strict mathematical formulas.

4. External electromagnetic field and electrons as a catalyst

Catalysis never ceases to amaze with the variety of types of catalytic reactions. In recent years, a number of publications have appeared in which catalytic reactions are considered using hydrated electrons instead of traditional catalysts [13–14].

Works on catalysis have appeared, in which, instead of a material catalyst, the influence of an external electric field on the acceleration of chemical reactions is studied [15–16]. In them, the acceleration of the reaction occurs without a catalyst only under the action of an electric field. According to the authors of [16], this opens the way to a fundamentally new type of catalysis, electrostatic catalysis. A new type of catalysis was observed using the Diels-Alder reaction as an example.

In [17], a new approach to the photocatalytic reduction of molecular nitrogen at low temperature and pressure using solvated electrons is presented. This new photocatalytic reduction paradigm is based on the transfer of electrons directly to the reactants.

As you can see, the scientific world is already approaching the understanding that material catalysts are not an obligatory attribute of catalysis. An immaterial substance - a field, and an elementary particle - an electron can act as a catalyst. This indicates that the role and place of catalysts in catalysis is not yet fully understood.

American chemists have found a condition under which catalysis using traditional catalysts proceeds at a rate significantly exceeding the Sabatier maximum [18–21]. This discovery became possible due to a special external influence on the catalyst, in which the catalyst passes from a static state into a dynamic state. An external influence causes a catalytic resonance and changes the activity of the catalyst so much that it causes it to increase the reaction rate beyond the capabilities of a traditional catalyst (above the Sabatier maximum). Studies have shown that the result of external action is a change in the electron density of the catalyst surface [18 – 23]. Thus, in this case too, the electrons are responsible for the excess of the reaction rate above the Sabatier maximum.

In recent years, the number of studies on the effect of external fields on the efficiency of catalysis has increased dramatically. In [24], a good review of methods for increasing the efficiency of catalytic reactions under various types of external action is presented.

As we can see, electrons are the most important active factor in heterogeneous catalysis, and the catalyst ensures their "correct" participation in catalysis. A substance can act as a catalyst as a carrier and supplier of electrons, as well as a field as an electron generator. Attributing fields to catalysts forces us to radically reconsider the modern concept of catalysis and look for new explanations for the mechanism of catalytic reactions.

5. Catalysts - carriers (generators) of the active factor of catalysis

Currently, many formulations of “what the catalyst is” have been voiced. It is usually said that the catalyst “is not part of the final products”, or “is not consumed during the reaction”, or “accelerates the chemical reaction, reducing its activation energy” [25, 26]. None of the known formulations gives an exhaustive definition of what a catalyst is. In these formulations there is no indication either of the mechanism by which the catalyst reduces the activation energy, or of the features of its structure that determine its catalytic activity, or of the characteristics of the catalyst substance that are capable of reducing the activation energy.

The IUPAC Golden Book defines it as follows: “A catalyst is a substance that increases the rate of a reaction without changing the overall standard change in the Gibbs energy of the reaction. A catalyst is both a reactant and a reaction product” [27]. In this formulation, there is also no indication of the features and characteristics of the catalyst substance that affect the reaction rate. But most importantly, a catalyst is defined as a substance. Recent studies have revealed a new type of physical influence on chemical reactions with the help of an external electric field, which is considered as a physical catalyst or pseudocatalyst [15, 24]. But since the field is not a reactant, not a product and not even a substance [15], the IUPAC formulation is also not a universal definition of a catalyst. The field, as a catalyst or pseudo-catalyst, is outside the scope of this IUPAC definition.

The abundance of different formulations and the lack of a unified and generalized definition of a catalyst indicates that the true role and mechanism of participation of a catalyst in a catalytic reaction is not yet fully understood. New ideas and a new approach are needed to determine the role and function of catalysts in catalytic reactions.

In [28, 29], a new concept of catalysis was proposed, within which catalysts are not considered as active factors of catalysis and are not considered as direct participants in catalytic reactions. Catalysts in this concept are given a different role - they are carriers (generators, suppliers) of the active factor of catalysis. The real participants, the real active factors of catalytic reactions are two elementary particles - an electron and a proton.

The main function of catalysts in catalytic reactions is to reduce the activation energy of the reaction. According to the new concept this is achieved by changing the oxidation state of the reactants. The change in the oxidation state of reactants in heterogeneous catalysis occurs with the participation of electrons. The determining action and the main mechanism of heterogeneous catalysis is the transfer of electrons from the catalyst to the reactant and from the reactant to the catalyst. This function of electron transfer is realized by catalysts in the mechanism of donor-acceptor interaction with reagents. In the course of the reaction, a cyclic change in the oxidation state of the catalysts occurs, which leads to a change in the oxidation state of the reactants (to a change in the redox state of the reaction medium). To do this, the catalysts themselves must have a special property. They must have the property of easily changing their oxidation state and easily perform the function of transmitting and receiving electrons. These are the main requirements for a catalyst. These requirements apply to both inorganic and organic catalysts [30, 31].

Thus, we consider the oxidation states of chemical elements as the most important characteristics of a substance for catalysis for all participants in the catalytic process

[28, 29]. These characteristics of the reagents and the catalyst substance, which are essential for catalysis, are well known in chemistry. They are included in reference books and are in the table of oxidation states of chemical elements [32].

The implementation of the donor function by the catalyst leads to the formation of negatively charged ions of the reagent. The implementation of the acceptor function by the catalyst leads to the formation of positively charged ions of the reagent. The resulting ions of one reactant meet opposite ions of the second reactant and enter into a chemical reaction with them. The reaction between ions requires a much lower activation energy than between molecules and proceeds much faster [33].

6. Laws of catalysis

The new concept of catalysis and a new approach to understanding the role and place of catalysts in catalytic reactions and the decisive role of electrons in the mechanism of catalysis confirmed in many studies, made it possible to obtain the basic laws of heterogeneous catalysis. The laws of catalysis take into account the role of the redox states of the catalyst and reactants and changes in their redox states. The laws of heterogeneous catalysis were obtained on the basis of the electron donor-acceptor mechanism of heterogeneous catalysis [28, 34, 35].

The 1-st law of catalysis (the law of catalysis rate) has the form [28, 34-36]:

$$v = \frac{e \bullet n_a \bullet |k_1 - k_2|}{F \bullet (\tau_D + \tau_A) \bullet m_1 \bullet |z_1 - z_2|}; \qquad (1)$$

where: v - is the rate of the catalytic reaction (mol/s); n_a *– the number of active sites of the catalyst involved in the reaction; F - is Faraday's constant; e - is the electric charge of the electron;* τ_D *- the time of the donor half-cycle of catalysis;* τ_A *- the time of the acceptor half-cycle of catalysis;* k_1 *- is the initial oxidation state of the catalyst;* k_2 *- is the final oxidation state of the catalyst;* z_1 *– the degree of oxidation of the reagent in the original product;* z_2 *– the degree of oxidation of the reagent in the final product;* m_1 *- is the number of reagent atoms in the final product molecule.*

From the 1-st law of catalysis directly follows the relation for calculating the yield of the catalytic reaction *(n)* [28]:

$$n = \frac{e \bullet n_a \bullet t \bullet |k_1 - k_2|}{F \bullet (\tau_D + \tau_A) \bullet m_1 \bullet |z_1 - z_2|}; \qquad (2)$$

where: t - is the time of the catalytic reaction.

The formula of the 1-st law of catalysis includes the key features of catalysis: a change in the oxidation state of catalysts and a change in the oxidation state of a reactant. The key role in catalysis is played by the cyclic frequency of the change in the redox state of the catalyst, which depends on the duration of the donor and acceptor half-cycles of catalysis. The productivity of catalysis depends on the intensity of the change in the oxidation state of the catalyst. The duration of the cycle of change in the redox state of the catalyst is determined by the time of electron transfer from the catalyst to the reagent and vice versa.

The 2-nd law of catalysis (conservation law) has the form [28]:

$$K_c \bullet n_a \bullet |k_1 - k_2| = n \bullet m_1 \bullet |z_1 - z_2| \bullet N_A = n \bullet m_2 \bullet |q_1 - q_2| \bullet N_A; \quad (3)$$

where: K_c *- the number of cycles of change in the state of oxidation of the active site of the catalyst;* m_1 *- is the number of atoms of the first reactant in the molecule of the final product;* m_2 *- is the number of atoms of the second reagent in the molecule of the final product;* q_1 *- the degree of oxidation of the second reagent in the original product;* q_2 *- is the degree of oxidation of the second reactant in the final product;* N_A *- Avogadro's number.*

Conservation law in catalysis: "*The product of the number of change cycles in the oxidation state of active sites of the catalyst by the number of sites and the amount of change in their oxidation state is equal to the product of the number of molecules of the final product by the number of reactant atoms in the molecule of the final product and the amount of change in the oxidation state of the reactant.*"

The 3-rd law of catalysis (the catalytic balance equation) has the form [36]:

$$N_{kat}^{red} + N_{kat}^{ox} = m_1 \bullet N_1^{red} + m_2 \bullet N_2^{ox}; \quad (4)$$

where: N_{kat}^{red} *- the number of elementary acts of catalyst recovery;* N_{kat}^{ox} *- the number of elementary acts of the catalyst oxidation;* N_1^{red} *- the number of elementary acts of recovery of the first reagent;* N_2^{ox} *- the number of elementary acts of oxidation of the second reagent;* m_1 *- is the number of atoms of the first reactant in the molecule of the final product;* m_2 *- is the number of atoms of the second reactant in the final product molecule.*

Elementary acts of oxidation-reduction lead to the formation of one molecule of the final product. The catalytic balance equation: *"the sum of the elementary acts of reduction and oxidation of the catalyst is equal to the sum of the elementary acts of oxidation and reduction of the reagents."*

Equations (1) and (2) can be represented as:

$$v = \frac{e \bullet n_a \bullet TOF}{F}; \quad (5)$$

$$n = \frac{e \bullet n_a \bullet TON}{F}; \quad (6)$$

Equations (1) and (2) include the most important characteristics of catalysis—the turnover frequency (TOF) of the catalytic reaction and the turnover number (TON) of the catalytic reaction. The relation for TOF and TON has the form [35 - 38]:

$$TOF = \frac{|k_1 - k_2|}{(\tau_D + \tau_A) \bullet m_1 \bullet |z_1 - z_2|}; \quad (7)$$

$$TON = \frac{|k_1 - k_2| \bullet t}{(\tau_D + \tau_A) \bullet m_1 \bullet |z_1 - z_2|}; \quad (8)$$

It was shown in [34] that the laws of catalysis are quantum laws. Using the example of the first law of catalysis, relation (1) can be represented as:

$$v = \frac{n_a \bullet \alpha \bullet \hbar \bullet c \bullet 4\pi\varepsilon_0 \bullet |k_1 - k_2|}{e \bullet F \bullet (\tau_D + \tau_A) \bullet m_1 \bullet |z_1 - z_2|}; \quad (9)$$

where: $\hbar$ *- Planck's constant,* α *- fine structure constant, e - electron charge, c - speed of light, F - Faraday's constant,* ε_0 *- dielectric constant.*

Formulas (7) and (8) are new formulas for calculating TOF and TON in addition to the relations known in catalysis [37, 38]:

$$TOF = \frac{n \bullet N_A}{t \bullet n_a}; \quad (10)$$

$$TON = \frac{n \bullet N_A}{n_a}; \quad (11)$$

where: N_A *- is Avogadro's number.*

Relations (7) and (10) and relations (8) and (11) are equivalent formulas for calculating TOF and TON:

$$TOF = \frac{n \bullet N_A}{t \bullet n_a} = \frac{|k_1 - k_2|}{(\tau_D + \tau_A) \bullet m_1 \bullet |z_1 - z_2|}; \ (12)$$

$$TON = \frac{n \bullet N_A}{n_a} = \frac{|k_1 - k_2| \bullet t}{(\tau_D + \tau_A) \bullet m_1 \bullet |z_1 - z_2|}; \ (13)$$

As shown in [37, 38], TOF is not a complete and unambiguous characteristic of a catalyst. Instead of TOF as a measure for comparing the activity of catalysts, it was proposed to use another characteristic, the frequency of changes in the redox state of the catalyst (redox frequency (ROF)). We call this characteristic the redox frequency of the catalyst or the turnover frequency of the catalyst. The ROF value can be calculated in two ways [39]:

$$ROF = \frac{n \bullet N_A \bullet \sigma}{t \bullet n_a} = \frac{1}{\tau_D + \tau_A}; \ (14)$$

where: σ *- is Horiuchi stoichiometric number [40].*

By analogy with TON, a new characteristic for the catalyst can be introduced - the number of changes in the redox state of the catalyst (redox number (RON)) [39]. We call this characteristic the number of revolutions of the catalyst:

$$RON = \frac{n \bullet N_A \bullet \sigma}{n_a} = \frac{t}{\tau_D + \tau_A}; \quad (15)$$

The 1-st and 2-nd laws of catalysis can be represented using ROF and RON. The ratios will look like:

$$v = \frac{e \bullet n_a \bullet ROF}{F \bullet \sigma}; \ (16)$$

$$RON \bullet n_a \bullet |k_1 - k_2| = n \bullet m_1 \bullet |z_1 - z_2| \bullet N_A = n \bullet m_2 \bullet |q_1 - q_2| \bullet N_A; \ (17)$$

The formula for calculating the yield of a catalytic reaction using RON is:

$$n = \frac{e \bullet n_a \bullet RON}{F \bullet \sigma}; \quad (18)$$

The value of the Horiuchi stoichiometric number depends on the change in the oxidation state of the catalyst and reactants and is determined in two ways:

$$\sigma = \frac{m_1 \bullet |z_1 - z_2|}{|k_1 - k_2|} = \frac{m_2 \bullet |q_1 - q_2|}{|k_1 - k_2|}; \quad (19)$$

The Horiuchi stoichiometric number and RON allow us to obtain a compact formula and a compact definition of the 2-nd law of catalysis [39]:

$$RON \bullet n_a = n \bullet N_A \bullet \sigma; \quad (20)$$

Conservation law in heterogeneous catalysis: *"The product of the number of catalyst turnovers by the number of active sites is equal to the product of the number of molecules of the final product by the Horiuchi number".*

The laws of heterogeneous catalysis and the formulas of the laws are given in Table 1. Based on the laws of catalysis, Table 1 gives a new definition of catalysis.

Table 1. Laws of heterogeneous catalysis, formulas and definitions

Name	**Formula for catalysis law**	**Note**
1-st law of catalysis	$v = \frac{e \bullet n_a \bullet \lvert k_1 - k_2 \rvert}{F \bullet (\tau_D + \tau_A) \bullet m_1 \bullet \lvert z_1 - z_2 \rvert}$	Catalysis rate law
2-nd law of catalysis	$RON \bullet n_a = n \bullet N_A \bullet \sigma$	Conservation law in catalysis
3-rd law of catalysis	$N_{kat}^{red} + N_{kat}^{ox} = m_1 \bullet N_1^{red} + m_2 \bullet N_2^{ox};$	Catalytic balance equation
Catalysis	*Catalysis - is the initiation or acceleration of a chemical reaction in the presence of a catalyst by reducing its activation energy by changing the oxidation state of the reactants during donor-acceptor or electromagnetic interaction of the catalyst with the reactants.*	

The three most important characteristics of heterogeneous catalysis (reaction yield (n), TOF, TON) and formulas for their calculation are given in Table 2.

Table 2. Characteristics of heterogeneous catalysis

Designation and name	**Formulas**	**Note**
n	$n = \frac{e \bullet n_a \bullet t \bullet \lvert k_1 - k_2 \rvert}{F \bullet (\tau_D + \tau_A) \bullet m_1 \bullet \lvert z_1 - z_2 \rvert}$	Yield of catalytic reaction

TOF (turnover frequency)	$TOF=\frac{n\bullet N_A}{t\bullet n_a}$; $TOF=\frac{\lvert k_1-k_2\rvert}{(\tau_D+\tau_A)\bullet m_1\bullet\lvert z_1-z_2\rvert}$	Turnover frequency of the catalytic reaction; donor-acceptor interaction constant
TON (turnover number)	$TON=\frac{n\bullet N_A}{n_a}$; $TON=\frac{\lvert k_1-k_2\rvert\bullet t}{(\tau_D+\tau_A)\bullet m_1\bullet\lvert z_1-z_2\rvert}$	The number of revolutions of the catalytic reaction

The oxidation states of the reactants, the oxidation states of the active sites of the catalyst, the Horiuchi number and the form of their entry into the laws of catalysis are given in Table 3.

Table 3. The oxidation states of the catalyst and reagents in the formulas of the laws of catalysis

Designation	**As represented in the laws of catalysis**	**Note**
k_1, k_2	$\lvert k_1-k_2\rvert$	Catalyst oxidation states
z_1, z_2	$\lvert z_1-z_2\rvert$	Oxidation states of the first reactant
q_1, q_2	$\lvert q_1-q_2\rvert$	The oxidation states of the second reactant
σ	$\sigma=\frac{m_1\bullet\lvert z_1-z_2\rvert}{\lvert k_1-k_2\rvert}$ $\sigma=\frac{m_2\bullet\lvert q_1-q_2\rvert}{\lvert k_1-k_2\rvert}$;	Horiuchi stoichiometric number

7. Catalysis is a fundamental physical and chemical phenomenon

The above laws of heterogeneous catalysis inspire confidence that catalysis is not a set of empirical techniques and not an art, but a fundamental physical and chemical phenomenon based on a fundamental physical interaction. The fundamental status of catalysis has many confirmations. One confirmation is that the main participant in the catalytic reaction is the electron. An electron in quantum physics is defined as a fundamental particle. The second confirmation is that the laws of catalysis include fundamental physical constants - elementary electric charge (e), Faraday's constant (F), Avogadro's number (N_A). The third confirmation is that the donor-acceptor interaction in catalysis is a special case of electromagnetic interaction - one of the 4 fundamental interactions in nature. The fourth confirmation is that the laws of catalysis are obtained on the basis of the fundamental physical law of conservation - the law of conservation of electric charge. The laws of heterogeneous catalysis have all the characteristics of quantum laws and belong to the class of laws of quantum chemistry and quantum electrodynamics. By analogy with the fundamental physical laws, the formulas of which necessarily include the interaction constant, the donor-acceptor interaction constant (TOF) is also defined for the laws of catalysis, which is included in the mathematical formulas of the laws of catalysis.

Note that what was said above about the fundamental status of heterogeneous catalysis can also be extended to homogeneous catalysis. The proton, as the main participant in homogeneous catalysis, is a fundamental particle. In homogeneous catalysis, a proton donor-acceptor mechanism of proton transfer and acceptance by the catalyst is implemented. The donor-acceptor interaction is a particular case of the fundamental electromagnetic interaction. The proton has the same elementary electric charge (e), which is a fundamental physical constant. In homogeneous catalysis, a fundamental law of conservation operates - the law of conservation of electric charge. Therefore, catalysis, as a fundamental phenomenon, can be safely attributed to the field of exact science, and not to art.

Catalysis, by its nature, refers to electrochemical processes, where the laws of quantum chemistry and quantum electrodynamics apply. In table 4 for comparison is shown the place of the laws of catalysis in the family of the most important fundamental physical laws.

Table 4. Laws of catalysis and fundamental physical laws

	Law of gravity	**Coulomb's law**	**Faraday Laws of electrolysis**	**Ohm`s Law**	**Laws of catalysis**
Type of interaction	Gravitational	Electro-magnetic	Electro-magnetic	Electro-magnetic	Donor-acceptor
Characteristic	Force (*F*)	Force (*F*)	Performance (n_F)	Current (*I*)	Catalysis reaction speed (*v*)
Law Formula	$F = G\frac{m_1 \bullet m_2}{r^2}$	$F = k\frac{q_1 \bullet q_2}{r^2}$	$n_F = \frac{I \bullet t}{F \bullet z_1}$	$I = \frac{U}{R}$	$v = \frac{e \bullet n_a \bullet TOF}{F}$ $RON \bullet n_a = n \bullet N_A \bullet \sigma$ $N_{kat}^{red} + N_{kat}^{ox} = m_1 \bullet N_1^{red} + m_2 \bullet N_2^{ox}$
nteraction constant	*G*	*k*	*F* (Faraday constant)	*R*	*TOF*
Interaction constant formula		$k = \frac{1}{4\pi\varepsilon_0}$	$F = e \bullet N_A$	$R = \frac{\rho \bullet l}{S}$	$TOF = \frac{\lvert k_1 - k_2 \rvert}{(\tau_D + \tau_A) \bullet m_1 \bullet \lvert z_1 - z_2 \rvert}$
The value of the interaction constant	From formula: $G = \frac{F \bullet r^2}{m_1 \bullet m_2}$	From formulas: $k = \frac{F \bullet r^2}{q_1 \bullet q_2}$	From formulas: $F = \frac{I \bullet t}{n_F \bullet z_1}$ $F = e \bullet N_A$	From formulas: $R = \frac{U}{I}$ $R = \frac{\rho \bullet l}{S}$	From formulas:

		$k = \frac{1}{4\pi\varepsilon_0}$			$TOF = \frac{N}{t \bullet n_a}$ $TOF = \frac{\lvert k_1 - k_2 \rvert}{(\tau_D + \tau_A) \bullet m_1 \bullet \lvert z_1 - z_2 \rvert}$
Theory	Gravitation theory	Electromagnetic theory	Electrolysis theory	Electric circuit theory	Donor-acceptor theory of catalysis

Table 4 clearly shows that the laws of catalysis have much in common with fundamental physical laws known in science. The laws of catalysis have all the signs of a fundamental status and complement the family of the most important laws of Nature.

8. Fundamental status of TOF in catalysis

In [37, 38], emphasis was put on the need to revise the status of TOF in catalysis. Studies have shown that TOF is more than a catalyst performance. TOF does not refer to a catalyst, but to the “catalyst + reagents” system, and its substantial essence is directly related to the mechanism of catalysis. As follows from Table 4, TOF plays the role of an interaction constant in the laws of catalysis. The fundamental status of the laws of catalysis and the inclusion of TOF in the formulas of the laws of catalysis as an interaction constant indicates the fundamental status of TOF in catalysis. TOF, as the turnover frequency of a catalytic reaction, claims to be an integral characteristic of catalysis process, taking into account the donor-acceptor interaction of the catalyst with the reagents. Therefore, we define TOF as the constant of the donor-acceptor interaction in the laws of catalysis.

9. Catalytic force of Berzelius

Berzelius defined catalysts as substances that have a mysterious catalytic power. In his doctrine of catalysis, the catalytic force that causes substances to react is defined as "a universal force inherent in both organic and inorganic nature" [26]. Berzelius at that time did not and could not give an explanation of the nature of the catalytic force. However, he pointed out that "the catalytic force must consist in some influence on the polarity of the atoms which it increases, decreases or changes so that in fact it is based on the excitation of electrical relations" [41]. We draw the reader's attention to the fact that Berzelius in his definition emphasized the electrical nature of the catalytic force.

Note that this was said by Berzelius in 1843 long (54 years!) before the discovery of the electron. It is clear why the doctrine of Berzelius's catalysis, due to the catalytic force that had no explanation in those years, was not accepted, but one cannot agree that his doctrine after the discovery of the electron in many publications is called metaphysical.

In the laws of catalysis obtained by us, we see the “materialization” of the metaphysical catalytic force of Berzelius in the form of an elementary particle – an electron. If we apply modern terminology to the above statement of Berzelius, then the catalytic power does not appear as a mystical power. It remains only to admire the foresight of Berzelius! He was ahead of his time! The price of this advance of time was the unreasonable attachment of a metaphysical label to his teaching. After the discovery of the electron (1897), it became possible to give a scientific explanation for Berzelius's catalytic power and to save it from metaphysical interpretation, but the catalytic gurus of the time could not benefit from this discovery.

The same cannot be said about Lowry, who immediately after the discovery of the proton put forward a new theory of acids and bases (the Bronsted-Lowry theory), and then in (1925 - 1928) developed the proton donor-acceptor mechanism as applied to homogeneous catalytic processes [42].

We noted above that new ideas and new approaches are needed to evaluate the role and function of catalysts in catalytic reactions. It turns out that the new idea turned out to be the long-forgotten old idea of Berzelius about the catalytic force, which is still undeservedly considered metaphysical. The discovery of the electron and proton revived Berzelius' theory of the catalytic force. The catalytic force now appears in the form of real material objects, in the form of elementary particles - an electron and a proton.

10. New definitions of catalysis and catalysts

Over the long history of catalysis its definition has changed many times, adjusting to different types of catalysis. The definition of catalysis has been repeatedly refined and supplemented, since the previous formulations did not reflect the current understanding of the essence of catalysis. Every time this was facilitated by the emergence of yet another “local” theory of catalysis. For example, in [43] 27 definitions of “what catalysis is” are given. It turned out that none of these 27 definitions is common to many types of catalytic reactions [26].

The most accurate and complete definition of catalysis was given by academician G.K. Boreskov, *“catalysis is the initiation or acceleration of chemical reactions in the presence of substances (catalysts) that repeatedly enter into intermediate chemical interaction with reagents and restore their chemical composition after each cycle of such interaction”* [1, 44].

As Romanovsky B.V. notes, this definition of catalysis also has drawbacks, it only describes the phenomenon of catalysis, without pointing out the physical causes that lead to the acceleration of chemical reactions and is phenomenological nature [1]. *“Such an approach is far from accidental and is characteristic of all known definitions of catalysis that can be found in educational and scientific literature”* [1].

The laws of catalysis and the new concept of catalysis make it possible to give a new definition of catalysis, which indicates the physical causes leading to the acceleration of chemical reactions, the mechanism of catalysis, and the type of fundamental interaction realized in catalysis. The new definition of catalysis is given in Table 1.

As for the definition of a catalyst, we believe that for a generalized definition it is necessary to extend the class of catalysts to a new material object - the field, to include in the definition the properties of a real and field catalyst, to indicate the mechanism of the catalyst's action on the reactants, and to indicate the type of fundamental interaction in which the catalyst and reagents.

In Table 5 shows the two most important characteristics of the catalyst (ROF and RON) obtained from the 1st and 2nd laws of catalysis, formulas for their calculation and a new definition of the catalyst.

Table 5. Characteristics of catalysts

Designation and name	**Formulas for catalyst characteristics**	**Note**
ROF (redox frequency)	$ROF = \frac{n \bullet N_A \bullet \sigma}{t \bullet n_a}$; $ROF = \frac{1}{\tau_D + \tau_A}$	Redox frequency

RON (redox number)	$RON = \frac{n \bullet N_A \bullet \sigma}{n_a}$; $RON = \frac{t}{\tau_D + \tau_A}$	Redox number
Catalyst	*Catalyst - is a substance or field that initiates or increases the rate of chemical reaction by changing the oxidation state of the reactants during the donor-acceptor interaction of a material catalyst with the reactants or during the electromagnetic interaction of the field with the reactants.*	

11. Conclusion

The real participants and acting factors of catalysis are two elementary particles – an electron and a proton. These elementary particles implement a single mechanism for accelerating chemical reactions based on the donor-acceptor mechanism of catalysis. The main function of catalysts, both material and field ones, is the supply (generation) of electrically charged particles and the change with their participation in the oxidation state of reagents. This mechanism makes it possible to reduce the activation energy of the reaction.

In the electron donor-acceptor mechanism of catalysis, a material catalyst, when interacting with reagents, acts as an electron donor and acceptor. At the same time, the catalyst (substance) itself remains unchanged and participates in the reaction only with its electrons. If the catalyst is an external field, then the donor-acceptor mechanism of catalysis is also realized. In this case, under the action of an external field, the role of an electron donor is performed by one of the reagents, and the role of an electron acceptor is performed by another reagent. As in the case of a real catalyst, an external field action changes the oxidation state of the reactants, which makes it possible to reduce the activation energy of the reaction. At the same time, the catalyst itself (field) remains unchanged and participates in the reaction only with its energy.

The presence of the Faraday constant in the laws of catalysis indicates a clear connection between two phenomena - catalysis and electrolysis. It was shown in [29, 34] that Faraday electrolysis is a special case of catalysis. Both catalysis and electrolysis are based on a single mechanism based on a change in the oxidation states of reagents during donor-acceptor or electromagnetic interaction.

The laws of heterogeneous catalysis and their comparison with fundamental physical laws allow us to conclude that catalysis belongs to the class of fundamental physical and chemical phenomena.

Temperature, pressure and concentration are not directly included in the equations of the laws of catalysis. However, they affect the parameters included in the formulas of the laws, namely, the oxidation states of the catalyst and reagents and the rate of electron transfer in the mechanism of donor-acceptor or electromagnetic interaction. Therefore, their influence in the laws of catalysis can be easily taken into account by introducing the appropriate coefficients of influence. For example, the influence of temperature in the laws of catalysis can be taken into account by introducing the temperature coefficient (TOF (TC_{TOF} [hz/°C]) by analogy, as is done for the resistance constant in Ohm's law. The effect of temperature on the resistance value in Ohm's law is taken into account by introducing the temperature coefficient of resistance (TCR [Ohm/ °C]) [45].

Berzelius made the greatest contribution to catalysis. He is not only the founder of this grandiose trend in chemistry, but also proposed a breakthrough theory of catalysis that was ahead of its time, based on electrical phenomena in catalytic reactions.

12. Conclusions

1. Three basic laws of heterogeneous catalysis were discovered, formulas of laws and ratios for calculating the main characteristics of catalysis and catalysts are given. The laws of catalysis have signs of a fundamental status and complement the family of the most important laws of Nature.

2. The most important characteristics of the catalyst substance and reagents, which are included in the laws of catalysis, are their oxidation states [28, 29, 46]. The oxidation states determine the values of the most important characteristics of catalysis. As the main tool in the selection of catalysts, it is necessary to use the list of oxidation states of chemical elements known in chemistry.

3. Substantiation of the fundamental status of catalysis is given. It is shown that the most important characteristic of TOF catalysis also has a fundamental status and is a constant of the donor-acceptor interaction in the laws of catalysis.

4. The most important characteristics of the catalyst substance and reagents, which are included in the laws of catalysis, are their oxidation states [28, 29, 46]. Oxidation

states set the values of the most important characteristics of catalysis and are parameters in the formulas of the laws of catalysis. As the main tool in the selection of catalysts, it is necessary to use the list of oxidation states of chemical elements known in chemistry.

5. From the laws of catalysis, new characteristics of the catalyst are obtained - redox frequency (ROF) and redox number (RON), which are proposed to be used as a measure of its activity instead of TOF and TON. Two ways of calculating ROF and RON are given.

6. Based on the laws of catalysis, a new definition of catalysis is given. A new definition of a catalyst is proposed, in which the class of material catalysts is extended to field catalysts.

7. Both material and field catalysts implement a single donor-acceptor mechanism of catalysis. Material catalysts participate in the reaction with their electrons. Field catalysts also participate in the reaction with electrons, with the only difference being that one of the reactants acts as an electron donor, and the second reactant becomes an electron acceptor.

8. The laws of catalysis can become the basis for creating a new quantitative theory of catalysis.

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