

## Fundamental principles of the evolutionary development of A.M. Butlerov's theory of chemical structure into the unified theory of the structure of chemical compounds

© Oleg S. Sirotkin,<sup>1\*+</sup> and Rostislav O. Sirotkin<sup>2</sup>

<sup>1</sup> School of Materials Science and Engineering. Kazan State Power Engineering University.  
Krasnoselskaya St., 51. Kazan, 420066. Tatarstan Republic. Russia.

Phone: +7 (843) 527-92-29. E-mail: [sirotkin-49@mail.ru](mailto:sirotkin-49@mail.ru)

<sup>2</sup> School of Materials Science and Engineering. Kazan State Power Engineering University.

Krasnoselskaya St., 51. Kazan, 420066. Tatarstan Republic. Russia.

School of Plastics Technology. Kazan National Research Technological University.

K. Marx St., 68. Kazan, 420015. Tatarstan Republic. Russia. E-mail: [rsir@mail.ru](mailto:rsir@mail.ru)

\*Supervising author; +Corresponding author

**Keywords:** chemistry, theory, unified model of chemical bonds, structure of chemical compounds, properties of chemical compounds, system of chemical bonds and compounds.

### Abstract

In this paper, the analysis of the current state of A.M. Butlerov's theory of chemical structure; the tendency of attracting less attention was noted, including attempts to diminish its fundamental importance in the formation of the individuality of chemical science and the formation of its theoretical foundations, which distinguish it from other natural sciences. The issue of fragmentation of chemistry into a variety of subsections (separate "chemistries"), which hinders the development of A.M. Butlerov's ideas and have led, among other things, to the absence in the list of Ministry of Education and Science of the Russian Federation Higher Attestation Commission of a scientific specialty aimed at the development of common theoretical foundations of chemistry, like "General chemistry" or "Theoretical foundations of chemistry". Based on the analysis of the main principles of A.M. Butlerov's theory of chemical structure and identification of reserves in their content, an attempt was made to evolve it into a unified theory of structure of chemical compounds (UThSChC). This theory develops the ideas of A. M. Butlerov, while shifting the focus from the fundamental development of the meaning of just "chemical structure" of the molecules (substances) in his theory onto the expression "the structure of chemical compounds". Therefore in UThSChC an attempt was made to formulate three basic theoretical principles defining not just the specifics of chemical structure of molecular substances, but the features of the *occurrence* (1), *structure of chemical compounds of elements* (2) and *properties* (3) of different chemical substances. This is necessary to identify the difference in the influence of chemical structure of elements' compounds (molecular and non-molecular, etc.) on characteristics of different classes of chemical substances. At the same time, the formulation of these three provisions of the UThSChC within the paradigm of multilevel organization of matter and substance is based on the assumption that a chemical substance in the form of a chemical compound of elements is considered as a closed material system characterised by fundamental distinctions from substances of physical and biological levels. It was also shown that, in accordance with the theory developed, the unity of the nature of chemical substances and the difference in their chemical structure and properties is revealed within a unified model of chemical bond and a system of chemical bonds, and homo- and heteronuclear compounds using the symbiosis of classical and quantum-chemical calculations of bond characteristics. The present paper represents the content of the talk given at mini-symposium “Butlerov Heritage – 17-18”.

### References

- [1] A. Azimov Brief history of chemistry. *Moscow: Mir*. **1983**. 187p. (russian)
- [2] V.I. Kuznetsov. Evolution of vision of main chemistry laws. *Moscow: Nauka*. **1967**. 310p. (russian)
- [3] P.M. Zorkiy. A critical look at the basic concepts of chemistry. *Russian chemistry journal*. **1996**. Vol.40. No.3. P.5-25. (russian)
- [4] Ya.A. Ugai. General and inorganic chemistry. *Moscow: Vysshaya shkola*. **1997**. 527p. (russian)

- [5] O.S. Sirotkin. Chemistry on the threshold of XXI century (On chemistry's place in modern world, individuality and unity of its fundamental principles). *Kazan: KSTU*. **1998**. 120p. (russian)
- [6] O.S. Sirotkin, Principles of unified chemistry (Unitarity as basis for formation of individuality, developing uniqueness and fundamentality of chemical science). *Kazan: Fen*. **2003**. 252p. (russian)
- [7] O.S. Sirotkin, R.O. Sirotkin. Theoretical principles of chemistry (individuality and unity). *Kazan: KSPEU*. **2004**. 168p. (russian)
- [8] O.S. Sirotkin, R.O. Sirotkin, A.M. Trubacheva. On the necessity and procedure of taking into account the metallic component of a heteronuclear bond. *Russian Journal of Inorganic Chemistry*. **2005**. Vol.50. No.1. P.67-71.
- [9] O.S. Sirotkin, R.O. Sirotkin, P.B. Shibaev. Effect of the character of homo- and heteronuclear chemical bond on the intermolecular interaction energy and properties of halogens and hydrogen. *Russian Journal of Inorganic Chemistry*. **2011**. Vol.56. No.7. P.1104-1108.
- [10] O.S. Sirotkin, R.O. Sirotkin, Unified model of chemical bonds and system, which unites them, as fundamental basis for new stage of development of A.M. Butlerov's theory of chemical structure of substance. International Congress on Organic Chemistry dedicated to the 150-th anniversary of the Butlerov's Theory of Chemical Structure of Organic Compounds. September 18-23. **2011**. *Kazan, Russia*. Book of Abstracts. P.73.
- [11] O.S. Sirotkin, Evolution of A.M. Butlerov's theory of chemical substance structure into unitary theory of structure of chemical substances. *Moscow: INFRA-M*. **2013**. 272p. (russian)
- [12] O.S. Sirotkin, R.O. Sirotkin, Transformation of structure and properties of homo- and heteronuclear compounds upon variation of their chemical composition and bond between the elements. XX Mendeleev Congress on general and applied chemistry. Five-volumes book. Vol. 1: abstracts. *Ekaterinburg: Ural Branch of the Russian Academy of Sciences*. **2016**. P.347.
- [13] O.S. Sirotkin, R.O. Sirotkin, Chemistry (Principles of unified chemistry). *Moscow: KNORUS*. **2017**. 364p. (russian)
- [14] G.D. Sproul. Electronegativity and Bond Type: I. Tripartite Separation. *Journal of Chemical Education*. **1993**. Vol.70. P.531-534.
- [15] G.D. Sproul. Electronegativity and Bond Type: II. Evaluation of Electronegativity Scales. *Journal of Physical Chemistry*. **1994**. Vol.98. P.6699-6703.
- [16] G.D. Sproul. Electronegativity and Bond Type: III. Origins of Bond Type. *Journal of Physical Chemistry*. **1994**. Vol.98. P.13221-13224.
- [17] G.D. Sproul. Electronegativity and Bond Type. *Journal of Chemical Education*. **2001**. Vol.78. No.3. P.387-390.
- [18] G. Salas-Banueta, J. Ramirez-Vieyra, Ionico, covalente y metalico. *Educ. Quim*. **2010**. V. 21. № 2. P. 118-125.
- [19] W.B. Jensen, Logic, History, and the Chemistry Textbook. *Journal of Chemical Education*. **1998**. Vol.75. P.817-828.
- [20] N.L. Glinka, General chemistry. *Moscow: KNORUS*. **2010**. 752p. (russian)
- [21] R.O. Sirotkin, Electronic-nuclear, molecular and supramolecular structure of polymer materials and their physico-mechanical properties ('Composition – bond type – properties' in polymers and metals). *Kazan: KSPEU*. **2007**. 240p. (russian)
- [22] A.M. Butlerov. Introduction to comprehensive study of organic chemistry. Kazan. 1864. Essays. *Moscow: Academy of Sciences of the USSR*. **1955-1958**. (russian)
- [23] O.S. Sirotkin. Integral and differential principles of unitary concept of natural science (Paradigm of multilevel organisation of matter as natural basis of variety and unity of nature of objects of system of a Universe). *Kazan: KSPEU*. **2011**. 268p. (russian)
- [24] Yu.I. Solovyov, V.I. Kurashov. Chemistry at the crossroads of science: Historical process of interaction between natural sciences. *Moscow: Science*. **1989**. 192p. (russian)
- [25] L. Pauling. The nature of the chemical bond. *Moscow-Leningrad: Goskhimizdat*. **1947**. 440p. (russian)
- [26] O.S. Sirotkin, R.O. Sirotkin. On the possibility of assessment of a bond covalent (metallic) character in metal-covalent mono- and polymer homocompounds. Works of the 43<sup>rd</sup> Republican scientific conference. *Kazan: KECI*. **1991**. P.12-13. (russian)
- [27] O.S. Sirotkin, R.O. Sirotkin. Unified model of chemical bond between elements and the system, which unites basic homo- and heteronuclear chemical compounds. XX Mendeleev Congress on general and applied chemistry. Five-volumes book. Vol. 1: abstracts. *Ekaterinburg: Ural Branch of the Russian Academy of Sciences*. **2016**. P.322.

- FUNDAMENTAL PRINCIPLES OF THE EVOLUTIONARY DEVELOPMENT OF A.M. BUTLEROV'S THEORY... 13-31
- [28] O.S. Sirotkin, R.O. Sirotkin, Multilevel structure and properties of metals and polymers within the unified model of chemical bond. *Journal of Materials Science and Engineering A*. **2016**. Vol.6. No.2. P.71-74.
- [29] R.O. Sirotkin, O.S. Sirotkin. Chemical bond. *Kazan: KSPEU*. **2010**. 52p. (russian)
- [30] O.S. Sirotkin, D.V. Glukhov, R.R. Nazmutdinov. Quantum-mechanical assessment of metallic component of homonuclear chemical interaction. *Herald of universities. Chemistry and chemical technology*. **2004**. Vol.47. Iss.8. P.149-154. (russian)
- [31] O.S. Sirotkin, A.M. Trubacheva, D.V. Glukhov, R.O. Sirotkin. On possibility of developing a universal method of assessment of ratio of basic components of homo- and heteronuclear chemical interaction. *Materials of IX all-Russia conference «Structure and dynamics of molecular systems»*. Ufa: USC RAS. **2002**. Vol.2. P.132-136. (russian)
- [32] O.S. Sirotkin, R.O. Sirotkin, A.M. Trubacheva. Classical and quantum approaches to developing a unified model of chemical bond. *XVII Mendeleev congress on general and applied chemistry*. **2003**. Казань. Vol.2(A). P.328. (russian)
- [33] R.O. Sirotkin, O.S. Sirotkin, I.V. Ivshin et al. Titanium chemical nature features, which determine its most important performance properties in linear engine-generator. *ARPJ Journal of Engineering and Applied Sciences*. **2016**. Vol.11. No.16. P.9664-9666.
- [34] O.S. Sirotkin, R.O. Sirotkin. Collectivised electrons and a character of their localisation-delocalisation within the framework of the unified model of chemical bond. *Herald of Kazan technological university*. **2012**. No.4. P.17-22. (russian)
- [35] O.S. Sirotkin, R.O. Sirotkin, Fundamental principles of a new stage of development of A.M. Butlerov's theory of organic compounds' chemical structure. *Herald of technological university*. **2014**. No.17. P.39-44. (russian)
- [36] Ye.V. Babaev. Is the periodic system of molecules possible? A.P. Rudenko (Ed.). History and methodology of natural sciences: Philosophical issues of chemistry. Iss. 35. *Moscow: MSU*. **1988**. 216p. (russian)
- [37] E.V. Babaev, R. Hefferlin, Concepts of Periodicity and Hyper- periodicity: from Atoms to Molecules. Concepts in Chemistry, D.H. Rouvray, E.C. Kirby, Ed. *London: Research Studies Press Limited*. **1996**. P.24-81.
- [38] O.S. Sirotkin, R.O. Sirotkin, A.M. Trubacheva. Characteristics of homo- and heteronuclear bonds of fine electronic-nuclear structure and their effects on properties of metallic and nonmetallic materials. *Kazan: KSPEU*. **2009**. 302p. (russian)