# The problem of geometrization of the language of chemistry

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## ABSTRACT

A system of three starting hypotheses, concerning the different evolutionary stages in the development of scientific branches and sciences is formulated. Using these hypotheses the particular problem for geometrization of the language of chemistry is formulated and grounded in a general form. The way for solving this problem is outlined by formulating a system of four basic problems to be solved during the next evolutionary stage of the development of the language of chemistry. Several aspects of these system of problems are briefly discussed in order to clarify their meaning and to introduce the main context needed. The main results, presented in detail in the monograph [1], are briefly reviewed.

## INTRODUCTION

The problem of geometrization of the language of chemistry, to the best of our knowledge, has been formulated, grounded and partially solved for the first time in [1]. This state of the art is the reason for publications in this topic to be lacking till now. This fact indicates that the large number of problems, related to investigation of the logical structure of the language of chemistry and the logically correct definition of its notions and relations, as well as to the formalization and the mathematical modeling of these notions and relations, has been ignored so far with the result that the problem of geometrization of the language of chemistry has not been formulated and, even less, solved. It is clear that the solution of aforesaid problems is very important for the development and the progress of the language of every science, including that of chemistry. To our opinion, these problems have been ignored due partially to the theoretical chemistry being so far strongly and continuously concentrated mainly on studying the relationships between the structure of chemical notions and that of quantum physics. Thus, the simplified opinion that the theoretical chemistry is just applied quantum mechanics is now commonly accepted. This opinion, however, is not only quite simplified and rather is totally wrong. We are going to demonstrate this point of view in several papers.

The main aims of this paper are: (1) to formulate and ground the problem of geometrization of the language of chemistry in a general form and to outline the way of its solution in a set of four basic problems; (2) to present briefly some results discussed in detail in [1].

## FORMULATION AND GROUNDING OF THE PROBLEM: THREE BASIC EVOLUTIONARY HYPOTHESIS

One general concept for the existence of qualitatively differing evolutionary stages in the development of the scientific knowledge is formulated in [1]. This conception enables to formulate in a general form and to ground strictly enough the more particular problem for geometrization of the language of chemistry. That is why in order to formulate and ground this problem we shall formulate some of the basic hypothesis in this evolutionary concept and clarify the meaning of some notions.

The evolution of the scientific cognition about various groups of phenomena obeys rigorous laws, which can be found by analyzing the different evolutionary stages of the most developed sciences. The knowledge of these laws makes it possible to determine the main trends of developement for a science at a lower evolutionary stage. Even fragmentary, such a knowledge allows to formulate the main evolutionary problems to be solved for each less developed science during the forthcoming stage of its evolution. If we accept the aforesaid concept as a **first basic hypothesis**, and analyze the stages passed through by such sciences as geometry and physics, advanced in their evolution, we shall find that *the knowledge about the groups of phenomena studied by them has developed towards the creation of axiomatically formulated theories which describe the respective groups of phenomena in terms of entirely mathematical spatial concepts and models*. Let us accept as a **second basic hypothesis** that *this trend of development reveals one of the main laws directing the evolution of scientific knowledge*. Then, this law would also rule the development of chemistry. However, to the best of our knowledge, neither an axiomatically formulated theory describing the chemical phenomena through entirely mathematical spatial concepts and models has been proposed so far, nor the problem of the creation of such theories has been formulated in any detail. On the contrary, it is known that even D. Mendeleev, the discoverer of the periodic law, has thought it impossible to transform chemistry in a science like geometry [2]. Being overconcentrated on quantum mechanics the contemporary theoretical chemistry also totally ignores these problems.

In order to clarify the meaning of the aforesaid hypotheses we shall clarify the meaning of some important notions. So, by the term *axiomatization* one usually means *the process of investigation of the logical structure of a given scientific language, the correct formulation of its notions and relations, as well as the construction of axiomatic formulations of the different systems of logically consentient and non-contradictory statements of this science*. By formulating the problem of axiomatization of a given scientific language it enters, in fact, the highest evolutionary stage, reached so far by the most developed sciences [3]. On the other hand, the term *geometrization* means usually *such a reformulation of the statements of a given science that uses entirely mathematical spatial notions and models*. It should be accentuated that the geometrization of a given scientific language is impossible without its preliminary axiomatization. At the same time, the geometrization facilitates substantially the further axiomatization of the corresponding scientific language. In brief, these two processes are inextricably bound up each other and we consider them as being parts of one and the same process. We refer to this process later on as ***geometrization*** and define by this generalized term *the process of transformation of the language of a given science in a set of such axiomatic formulations of the systems of logically consentient and non-contradictory* *statements of this science that is characterized by a large-scale use of entirely mathematical notions and models*. By this generalized term we have tried to denote shortly and to point the main trend in the development of each science during a given strictly specified evolutionary stage referred to us as *the stage of geometrization of the language of this science*.

It is clear from the above said that the concept of geometrization of a given scientific language should be regarded in the most general sense of the term *geometry*. Classical examples for a final result of completed geometrization in the generalized meaning of this term are the formulations of different kinds of geometry [4, 5, 6, etc.]. Examples for well advanced geometrization are the mathematical formulations of many physical disciplines such as classical and quantum mechanics, thermodynamics, theory of relativity, electrodynamics, etc. [7, 8, 9, etc.].

Thus, if our two basic hypotheses are true, chemistry is still on a lower stage of development as compared to geometry and physics. So, as a **third basic hypothesis** we accept that *the main evolutionary problem for the contemporary chemistry is the problem of geometrization of its language in the above mentioned meaning*. By formulating and solving this problem chemistry enters a qualitatively new stage of development, namely the stage of its geometrization.

As a matter of fact, the problem of geometrization of the language of chemistry is a huge problem, the solution of which requires the sustained efforts of lots of researchers. We think, however, that the moment is ripe for this problem to be submitted for discussion, and this is the main aim of the present work.

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## OUTLINING OF THE WAY OF GEOMETRIZATION OF CHEMISTRY

Up to here we have formulated and grounded in a general form the problem of geometrization of the language of chemistry. Now, we shall trace out, in general, the way to solve it. It is clear from the definition of the generalized notion geometrization that to solve this problem one should find the solution of the following *system of four basic problems*, inextricably bound up with each other:

**1.** To reveal the logical structure of the language of chemistry in order to formulate correctly the chemical notions and relations;

**2.** To construct entirely mathematical spatial representations of these notions and relations;

**3.** To formulate systems of logically consentient, non-contradictory and veracious chemical statements playing the role of axiomatics in further axiomatic formulations of the language of chemistry;

**4.** To prove logically the truth of those chemical statements which are not axioms, i.e. these statements to be deduced from the formulated chemical axiomes.

Several aspects of the aforesaid problems require a brief discussion in order to clarify their meaning and to introduce the context main needed:

- The structure of basic chemical notions and relationships cannot yet be considered as entirely completed. This fact is illustrated by the existence and the continuous appearance of numerous nonequivalent representations of the Periodic law [10, 11, 12, etc.]. Thus, the mathematical modeling of the structure of basic chemical notions and relationships must start by the analysis of the logical structure of the language of chemistry. On the other side, due to the strong relation between the basic notions of each science, the mathematical modeling of every well-defined basic notion simplifies to a great extent the analysis of the logical structure of the language of this science and the correct definition of all other notions therein.

- Even a cursory analysis [1] shows that the current language of chemistry is logically imperfect. For example, there are considerable omissions, meaning anachronisms, a number of basic chemical notions are neither defined explicitly nor correctly and, in some cases, there are important differences between the definitions used by different authors[1]. In general, the language of chemistry is logically structureless and there is no a clear separation between the basic and derivative notions. It should be noted that logical imperfections are normal for scientific languages undergoing transition from a “lower, inductive stage” to a ”higher, deductive stage” and to ”the most higher (supreme), axiomatic stage” of its evolution [3]. Therefore, the elimination of these imperfections is one of the basic problems to be solved during the deductive and axiomatic stages of development of a science.

- The problem of the logical investigation and the correct formulation of a particular structure of scientific notions and relations is closely related to the problem of its mathematical modeling. That is why both problems should be solved simultaneously.

- The formulation and the solution of these problems enables the transition of chemistry from a lower inductive stage to a higher deductive stage of its evolution.

- Though new for chemistry, the problems of the logical investigation, the correct formulation and the mathematical modeling of a particular structure of notions and relations are well known for mathematics and logics. That is why, by formuling of these problems, the language of chemistry is “set in the context” of mathematics and logics.

- Adequate logical and mathematical tools must be used for solving the aforesaid problems. These include: explicit and correct formulation of different notions and statements of scientific language under study; use of tools such as the axiomatic method, mathematical modeling, etc.; use of logical classificational categories such as definition, axiom, theorem, lemma, corollary, etc.; introduction of adequate symbols for the notions of this system, and so on.

- Particular objects of the same *species*[2] are not subject of chemistry because of their equivalence. In other words, the *principle of equivalence*, known in quantum mechanics, holds also in chemistry. It should be noted that this principle, in general, is one of the basic axioms in the scientific knowledge.

- It is evident from the last comment that subjects of chemistry are sets of equivalent objects, rather than particular elements of these sets. Thus, *the category* ***species*** *is the basic classificational category in chemical taxonomy* (that is why common for chemistry is the usage of notions such as *species* of atoms, *species* of ionized atoms, *species* of polyatomic ions, *species* of molecules, etc.), and an extended exploitation of the theory of sets is necessary to geometrization of chemistry.

The complete solution of the aforesaid system of basic problems is by no means an easy task in both its large scale and variety. So, in the study performed [1] we confined ourselves to find out such rigorous partial solutions to the first three problems that would demonstrate that the problem of the geometrization of chemistry is solvable.

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## SUMMARY OF THE MAIN RESULTS

The main results presented in detail in [1] are:

**1)** A brief analysis was carried out of the logical structure of the fundamentals of chemistry. It was found out that they can be separated into four parts, in each of which a corresponding group of basic chemical notions was introduced. (See [13].)

**2)** A method for forming spatial mathematical representations of the basic chemical notions and relationships was developed.

**3)** Using this method we have constructed and analyzed one *approximate* and two *more precise* spatial mathematical models of *the set* **S** *of different species of atoms* which are at the same time mathematical models of three different tabular forms of the Periodic System. (See [13].)

**4)** In constructing the *approximate model* $\mathbf{P}=f(\mathbf{S},\mathbf{T_0})$ we started from a *simplified* tabular short form of the Periodic System, denoted as $\mathbf{T_0}$. This table represents only the most general characteristics of the Periodic law (*i.e.* the ordering of chemical elements in groups and periods, as well as the ordering of the groups and the periods), but does not represent the atoms of chemical elements belonging to the corresponding A or B subgroups. In constructing and analyzing the approximate model we have achieved the following goals: **(i)** the main concepts and the most significant mathematical elements, necessary for the construction of the more precise mathematical models of the basic chemical notions and relationships, were introduced; **(ii)** the developed method was demonstrated. Briefly, by the approximate model we have introduced and demonstrated the main part of tools, necessary for the geometrization of the language of chemistry.

**5)** Using the developed method we have formulated and analyzed two more precise mathematical models $\mathbf{Q}=f_1(\mathbf{S},\mathbf{T_1})$ and $\mathbf{G}=f_1(\mathbf{S},\mathbf{T_2})$ of of the set **S** of different species of atoms and of the Periodic Law making use of two different 32-column tabular extended forms of the Periodic System, denoted as $\mathbf{T_1}$ and $\mathbf{T_2}$. (See [13].)

**6)** The following goals were achieved in constructing and analyzing the aforesaid three models:

- the definitions of some basic chemical notions were revised;
- a number of specific chemical-mathematical symbols were introduced;
- the three- and two-dimensional images were determined for a number of basic chemical notions (chemical element, group and period of PS, maximal stoichiometric valence, etc.);
- for each of the three models a corresponding set of statements of various logical ranks (definitions, axioms, lemmas, corollaries, *etc.*) was formulated;
- a comparative analysis was carried out of the three spatial mathematical models, **P**, **Q** and **G**.

**7)** Two spatial mathematical models $Q = F_1(S, \mathbf{T_1})$ and $G = F_1(S, \mathbf{T_2})$ of the *set* S *of different species of monoatomic ions* were constructed and analyzed. These two models generalized the two more precise mathematical models **Q** and **G** of the set **S** of different species of atoms for the case of an arbitrary species of simple chemical objects. (See [13].)

**8)** A preliminary design for the geometrization of the other three parts of the chemistry fundamentals was formulated. (See [13].)

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## CONCLUSIONS

The five constructed spatial mathematical models **P**, **Q**, **G**, Q and G are, in fact, a geometrization of the first part of the chemistry fundamentals – i.e. of the ***statics*** *of the* ***simple chemical objects***.

The general conclusion from the results obtained is that ***the proposed mathematical models and preliminary designs, although not solving the problem of the geometrization of chemistry in a final form, demonstrate both the solvability of this problem and the ways to search for its solution***. Thus, though partially, they confirm the correctness of the formulated three basic hypotheses. Full details of the study performed are presented in [1].

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**NOTES**

[1] The lack of notions for classifying chemical objects in presence or absence of *chemical structure* is an example of omission. The identification of the notion *species of atoms* with the notion *chemical element* is a typical example of meaningful anachronism in the language of contemporary chemistry. For example, incorrect are the definitions of *ionization*, *recombination* and the *oxidation number*.

[2] *Species* in this study means the *major subdivision* of a *genus* or *subgenus*, regarded as the *basic category* of *chemical classification*. This is in accordance with the Random House Webster's meanings: 1) Logic. a) one of the classes of things included with other classes in a genus. b) the set of things within one of these classes. 2) the major subdivision of a genus or subgenus, regarded as the basic category of biological classification, composed of related individuals that resemble one another, are able to breed among themselves, but are not able to breed with members of another species.

## REFERENCES

**[1]** Penev V. Tz., Geometrization of the Fundamentals of Chemistry, Sofia, Riva Publ. House, 1997, (in Bulgarian with an extended summary in English)

**[2]** Semishin V. I., The Mendeleev's periodic system of chemical elements, Moskva, Chimia, 1972

**[3]** Blanche Robert, L' axiomatique, Paris, Press universitaires de France, 1965

**[4]** Euclid, Elements

**[5]** Lobachevsky N. I., Geometrical researches on the theory of paralleles, 7-th eddition, Chicago, Open Court, 1914

**[6]** Hilbert D., Grundlangen der Geometrie, Leipzig und Berlin, Verl. und Druck von B. G. Teubner, 1930

**[7]** Einstein A., Grundzuge der Relativitatstheorie, 5. Aufl., Berlin, Akademie-Verl., 1970;

**[8]** Wheeler J. A., Einsteins Vision. Wie stehet es heute mit Einsteins Vision, alles als Geometrie aufzufassen?, Berlin, Springer, 1968

**[9]** Wheeler J. A., Geometrodynamics, New York, Academic Press, 1962

**[10]** Semishin V. I., Literature on the Mendeleev's Law of Periodicity, Moskva, Visshaya shkola, 1969

**[11]** Semishin V. I. and Z. F. Semishina, Literature on the Mendeleev's Law of Periodicity, Moskva, Visshaya shkola, 1975

**[12]** Godovikov A. A., The Mendeleev's periodic system and the force characteristics of elements, Novosibirsk, Nauka, 1981

**[13]** Penev V., L. Konstantinov, M. Marinov. 2000. Logical structure of the fundamentals of chemistry, conceptual schemes of its geometrization and spatial mathematical models of the sets of different species of simple chemical objects. - Academic Open Internet Journal, Volume 2 (2000), Part 2: Chemistry. (http://www.acadjournal.com/2000/v2/part2/p3/index.html; mirror is available through: http://www.clmc.bas.bg/vpenev/vpenev.htm)