

A NEW ALGEBRA FOR BALANCING SPECIAL CHEMICAL REACTIONS

Ice B. Risteski

Abstract. In this article are balanced only special chemical reactions which have non-unique coefficients, or so-called *continuum reactions*. For that kind of chemical reactions is made a completely new algebraic analysis by virtue of determined generators. Here treated chemical reactions possess atoms with fractional and integer oxidation numbers. Also, in this article are determined the necessary and sufficient conditions for solution of two old problems.

Keywords: algebra, chemical reactions, balancing, generators.

Introduction

Balancing chemical reactions is a delightful topic for students which have chemistry as a major subject of study (Risteski, 1990). Mass balance of chemical reactions is one of the most highly studied topics in chemical education. In fact, balancing chemical reactions provides an excellent demonstrative and pedagogical example of interconnection between *chemical principles* and linear algebra. In chemistry there are lots of so-called *methods* for balancing chemical reactions, but all of them have limited usage, because they hold only for some elementary chemical reactions. Actually, they are not methods, just particular procedures founded by virtue of experience, but without any formal criteria. A survey of the references which treat problem of balancing chemical reactions through the prism of chemistry is given in the previous author's research works (Risteski, 2007a; 2007b; 2008a; 2008b; 2009).

So-called *chemical methods* for balancing chemical reactions are inconsistent, because they consider chemical reactions on an informal way, which produces only fallacies and paradoxes (Risteski, 2010; 2011).

Most of current chemistry textbooks generally support the *ion–electron procedure* as the general balancing tool that best makes use of *chemical principles*. But, now logi-

cally this question arises: *what are chemical principles?* According to Risteski (2010) the best short answer to this question is: *'Chemical principles' are not defined entities in chemistry, and so this term does not have any meaning. They represent only a main generator for paradoxes. Actually, 'chemical principles' are a remnant of an old traditional approach in chemistry.*

Until second half of 20th century there was no mathematical method for balancing chemical reactions in chemistry, other than algebraic method. Chemists balanced simple particular chemical reactions using only change in oxidation number procedure, partial reactions procedure and other slightly different modifications derived from them. So-called *chemical principles* were an assumption of traditional chemists, who thought that the solution of the general problem of balancing chemical reactions is possible by use of chemical procedures. But, practice showed that the solution of the century old problem is possible only by using contemporary mathematical method (Risteski, 2007a).

Also, in (Risteski, 2010) the author emphasized very clearly, that *balancing chemical reactions is not chemistry; it is just linear algebra*. From a scientifically view point, *a chemical reaction can be balanced if only if it generates a vector space*. That is a necessary and sufficient condition for balancing a chemical reaction. This shows that chemical reaction must be considered as a formal whole, in a right sense of the word, if we like it to be balanced on a correct way. In opposite case, as it was done by the *chemical methods*, one obtains only absurd (Risteski, 2011).

Here, the considered chemical reactions belong to the class of chemical reactions with non-unique coefficients. These reactions we shall name *continuum reactions*. Why? Reason is very clear. Coefficients of these reactions one can reduce to the *generalized problem of continuum*.

In the next section will be solved two open problems from the theory of balancing chemical reactions. For that purpose were employed the well-known algebraic method for balancing chemical reactions and elementary theory of analytical inequalities. Three more complex reactions are balanced too.

Main results

Problem

Long time ago Melville (1932) proposed this chemical reaction



Solution

The chemical reaction (1) reduces to a system of linear equations

$$x_1 = 2x_4 + 2x_5 + 2x_6,$$

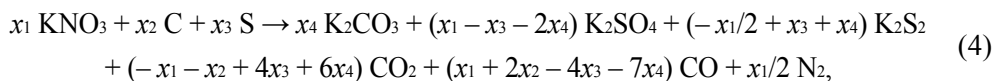
$$\begin{aligned}x_1 &= 2x_9, \\3x_1 &= 3x_4 + 4x_5 + 2x_7 + x_8, \\x_2 &= x_4 + x_7 + x_8, \\x_3 &= x_5 + 2x_6,\end{aligned}\tag{2}$$

which general solution is

$$\begin{aligned}x_5 &= x_1 - x_3 - 2x_4, \quad x_6 = -x_1/2 + x_3 + x_4, \\x_7 &= -x_1 - x_2 + 4x_3 + 6x_4, \\x_8 &= x_1 + 2x_2 - 4x_3 - 7x_4, \quad x_9 = x_1/2,\end{aligned}\tag{3}$$

where x_i , ($1 \leq i \leq 4$) are arbitrary real numbers.

If one substitutes (3) in (1), then the chemical reaction (1) becomes



where x_i , ($1 \leq i \leq 4$) are arbitrary real numbers.

The chemical reaction (4) is a four parametric reaction x_i , ($1 \leq i \leq 4$) with five generators $x_j > 0$, ($5 \leq j \leq 9$). These generators generate an infinity number particular cases of (4). Since, the generators $x_j > 0$, ($5 \leq j \leq 9$) then from (3) immediately follows this system of inequalities

$$\begin{aligned}x_1 - x_3 - 2x_4 &> 0, \\-x_1/2 + x_3 + x_4 &> 0, \\-x_1 - x_2 + 4x_3 + 6x_4 &> 0, \\x_1 + 2x_2 - 4x_3 - 7x_4 &> 0.\end{aligned}\tag{5}$$

From (5) one obtains the relations

$$x_2 < 2x_3 + 7x_4/2,\tag{6}$$

$$x_3 + 2x_4 < x_1 < 2x_3 + 2x_4.\tag{7}$$

The expressions (6) and (7) are necessary and sufficient conditions to hold the chemical reaction (4).

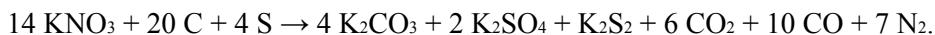
Now, the question arises: *How many points* $(x_1, x_2, x_3, x_4, x_1 - x_3 - 2x_4, -x_1/2 + x_3 + x_4, -x_1 - x_2 + 4x_3 + 6x_4, x_1 + 2x_2 - 4x_3 - 7x_4, x_1/2)$ *are there on the hypersurface in* \mathbb{R}^9 , *where* x_i , ($1 \leq i \leq 4$) *are arbitrary real numbers?* In other words, the question is: *How many different sets of integers do there exist?* (Gödel, 1947).

We shall build the reply to this question on the concept of the *continuum*. In fact, the word *continuum* is recognizable as the name used by Cantor to refer to the real line. From the expression (4), we can see that this kind of chemical reaction reduces to the *generalized Cantor's continuum problem*. That was the reason why we named these

reactions *continuum reactions*. This problem is simply condensed in the first question. This problem is neither simple nor easy; it needs a wide explanation. It shows that balancing chemical reactions is a main object in *Foundation of Chemistry*, which lies in an intertwined mixture of topology, abstract algebra, linear algebra, axiomatic set theory, mathematical logic, computability theory and proof theory.¹⁾

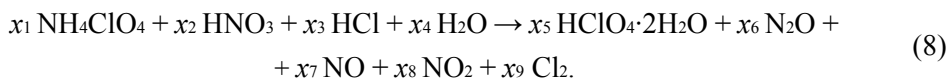
Example

Now, we shall consider this particular case of (4). For $x_3 = x_4 = 1$ from (6) one obtains $x_2 = 5$, while from (7) follows $x_1 = 7/2$. From (3) one obtains $x_5 = 1/2$, $x_6 = 1/4$, $x_7 = 3/2$, $x_8 = 5/2$ and $x_9 = 7/4$. Since, all the coefficients are determined then the balanced particular reaction has the form



Problem

As an unbalanced reaction Jensen (1987) proposed the reaction



Solution

First, we shall determine the general solution of (8). From (8) immediately follows a system of linear equations

$$\begin{aligned} x_1 + x_2 &= 2x_6 + x_7 + x_8, \\ 4x_1 + x_2 + x_3 + 2x_4 &= 5x_5, \\ x_1 + x_3 &= x_5 + 2x_9, \end{aligned} \quad (9)$$

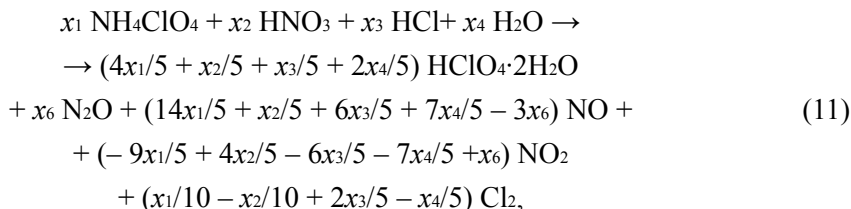
$$4x_1 + 3x_2 + x_4 = 6x_5 + x_6 + x_7 + 2x_8.$$

The general solution of the system (9) is given by these expressions

$$\begin{aligned} x_5 &= 4x_1/5 + x_2/5 + x_3/5 + 2x_4/5, \\ x_7 &= 14x_1/5 + x_2/5 + 6x_3/5 + 7x_4/5 - 3x_6, \\ x_8 &= -9x_1/5 + 4x_2/5 - 6x_3/5 - 7x_4/5 + x_6, \\ x_9 &= x_1/10 - x_2/10 + 2x_3/5 - x_4/5, \end{aligned} \quad (10)$$

where x_1, x_2, x_3, x_4 and x_6 are arbitrary real numbers.

If one substitutes (10) into (8), the chemical reaction (8) becomes



where x_1, x_2, x_3, x_4 and x_6 are arbitrary real numbers.

The reaction (11) is a five parametric reaction with four generators. Just these generators produce an infinity number particular cases of (11). Since, the generators $x_5, x_7, x_8, x_9 > 0$, then from (10) one obtains this system of inequalities

$$\begin{aligned} 4x_1 + x_2 + x_3 + 2x_4 &> 0, \\ 14x_1 + x_2 + 6x_3 + 7x_4 - 15x_6 &> 0, \\ -9x_1 + 4x_2 - 6x_3 - 7x_4 + 5x_6 &> 0, \\ x_1 - x_2 + 4x_3 - 2x_4 &> 0. \end{aligned} \quad (12)$$

From (12) immediately follow the relations

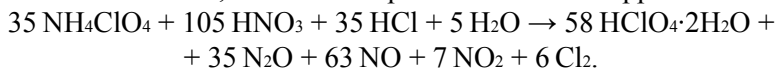
$$x_6 < (x_1 + x_2)/2, \quad (13)$$

$$-14x_1 - x_2 + 15x_6 < 6x_3 + 7x_4 < -9x_1 + 4x_2 + 5x_6. \quad (14)$$

The expressions (13) and (14) are necessary and sufficient conditions to hold the chemical reaction (11).²⁾

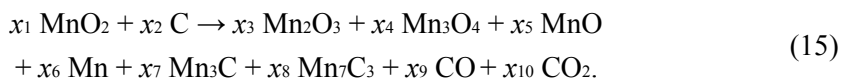
Example

Now, we shall consider a particular case of (11). For $x_1 = 1$ and $x_2 = 3$, from (13) one obtains $x_6 = 1$, while from (14) follows $x_3 = 1$ and $x_4 = 1/7$. For these particular values, from (10) one obtains $x_5 = 58/35$, $x_7 = 9/5$, $x_8 = 1/5$ and $x_9 = 6/35$. Since, all the coefficients are determined, the balanced particular reaction appears in the form



Problem

Now, we shall balance this chemical reaction



Solution

From the above reaction follows a system of linear equations

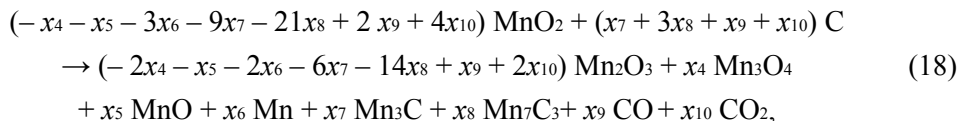
$$\begin{aligned} x_1 &= 2x_3 + 3x_4 + x_5 + x_6 + 3x_7 + 7x_8, \\ 2x_1 &= 3x_3 + 4x_4 + x_5 + x_9 + 2x_{10}, \\ x_2 &= x_7 + 3x_8 + x_9 + x_{10}. \end{aligned} \quad (16)$$

The general solution of the system (16) is

$$\begin{aligned} x_1 &= -x_4 - x_5 - 3x_6 - 9x_7 - 21x_8 + 2x_9 + 4x_{10} \\ x_2 &= x_7 + 3x_8 + x_9 + x_{10} \\ x_3 &= -2x_4 - x_5 - 2x_6 - 6x_7 - 14x_8 + x_9 + 2x_{10}, \end{aligned} \quad (17)$$

where $x_i > 0$, ($4 \leq i \leq 10$) are arbitrary real numbers.

The balanced reaction (15) has the form



where $x_i > 0$, ($4 \leq i \leq 10$) are arbitrary real numbers. Since $x_i > 0$, ($1 \leq i \leq 3$) are the generators of the reaction (15), then from the general chemical reaction (18) holds this system of inequalities

$$\begin{aligned}
& -x_4 - x_5 - 3x_6 - 9x_7 - 21x_8 + 2x_9 + 4x_{10} > 0, \\
& x_7 + 3x_8 + x_9 + x_{10} > 0, \\
& -2x_4 - x_5 - 2x_6 - 6x_7 - 14x_8 + x_9 + 2x_{10} > 0.
\end{aligned} \tag{19}$$

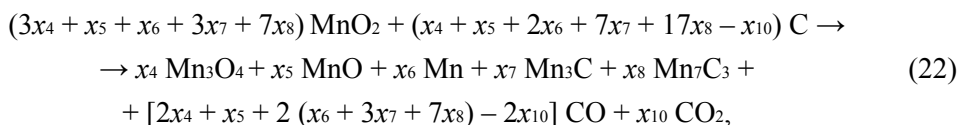
From (19) one obtains the inequality

$$x_9 + 2x_{10} > 2x_4 + x_5 + 2(x_6 + 3x_7 + 7x_8). \tag{20}$$

The inequality (20) is a necessary and sufficient condition to hold the general reaction (18). Now, we shall analyze the general chemical reaction (18). If

$$x_9 + 2x_{10} = 2x_4 + x_5 + 2(x_6 + 3x_7 + 7x_8), \tag{21}$$

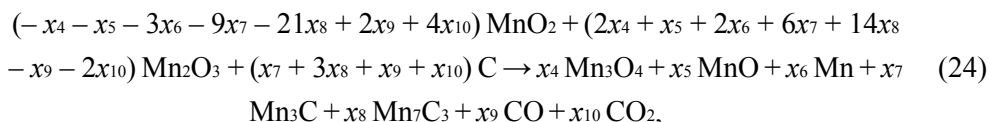
then from (18) follows



where $x_i > 0$, ($4 \leq i \leq 8$) and $x_{10} > 0$ are arbitrary real numbers. If

$$x_9 + 2x_{10} < 2x_4 + x_5 + 2(x_6 + 3x_7 + 7x_8), \tag{23}$$

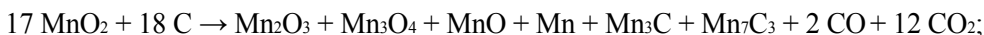
then from (18) one obtains



where $x_i > 0$, ($4 \leq i \leq 10$) are arbitrary real numbers.

As particular reactions of (18) we shall derive the following cases:

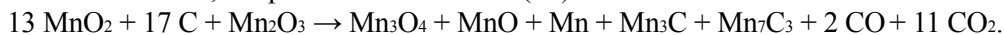
(i) For $x_4 = x_5 = x_6 = x_7 = x_8 = 1$, from (20) follows $x_9 + 2x_{10} > 25$, i. e. $x_9 + 2x_{10} = 26$. Let $x_9 = 2$, then $x_{10} = 12$. Now, from (17) one obtains $x_1 = 17$, $x_2 = 18$ and $x_3 = 1$. Thus, the particular reaction of (18) has these coefficients



(ii) For $x_4 = x_5 = x_6 = x_7 = x_8 = 1$, then from (21) follows $x_9 + 2x_{10} = 25$, such that for $x_9 = 5$, one obtains $x_{10} = 10$. Now, from (17) immediately follows $x_1 = 15$, $x_2 = 19$ and $x_3 = 0$. Thus, the particular reaction of (22) has this form

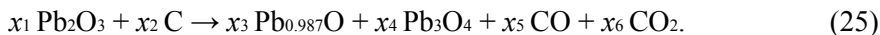


(iii) For $x_4 = x_5 = x_6 = x_7 = x_8 = 1$, from (23) we obtain $x_9 + 2x_{10} < 25$, i. e. $x_9 + 2x_{10} = 24$, then for $x_9 = 2$, one obtains $x_{10} = 11$. Now, from (17) we have $x_1 = 13$, $x_2 = 17$ and $x_3 = -1$. Thus, the particular reaction of (24) has these coefficients



Problem

Now, we shall balance this chemical reaction



Solution

From the above reaction follows this system of linear equations

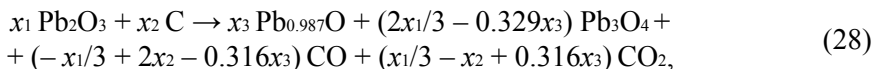
$$\begin{aligned} 2x_1 &= 0.987x_3 + 3x_4, \\ 3x_1 &= x_3 + 4x_4 + x_5 + 2x_6, \\ x_2 &= x_5 + x_6. \end{aligned} \quad (26)$$

The general solution of the system (26) is

$$\begin{aligned} x_4 &= 2x_1/3 - 0.329x_3, \\ x_5 &= -x_1/3 + 2x_2 - 0.316x_3, \\ x_6 &= x_1/3 - x_2 + 0.316x_3, \end{aligned} \quad (27)$$

where $x_i > 0$, ($1 \leq i \leq 3$) are arbitrary real numbers.

The balanced reaction has the form



where $x_i > 0$, ($1 \leq i \leq 5$) are arbitrary real numbers. Since x_4 , x_5 and x_6 are > 0 , then from (28) one obtains this system of inequalities

$$\begin{aligned} 2x_1/3 - 0.329x_3 &> 0, \\ -x_1/3 + 2x_2 - 0.316x_3 &> 0, \\ x_1/3 - x_2 + 0.316x_3 &> 0. \end{aligned} \quad (29)$$

From (29) one obtains the relation

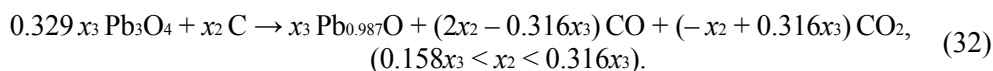
$$3x_2 - 0.948x_3 < x_1 < 6x_2 - 0.948x_3. \quad (30)$$

The relation (30) is a necessary and sufficient condition to hold the general chemical reaction (28). Now, we can analyze the general reaction (28) for all possible values of x_1 , x_2 and x_3 . As particular reactions of (28) we shall derive the following cases:

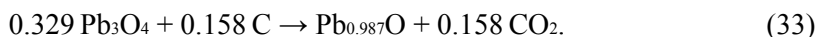
(i) For $x_1 = 3$, $x_2 = 2.4$ and $x_3 = 4.5$, from (27) follows $x_4 = 0.5195$, $x_5 = 2.378$ and $x_6 = 0.022$, i.e., one obtains this particular reaction



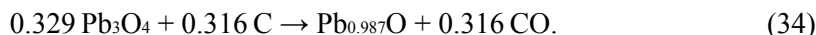
(ii) For $x_1 = 0$, from (28) one obtains this particular reaction



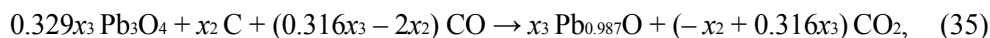
(iii) For $x_2 = 0.158 x_3$, from (32) one obtains



(iv) For $x_2 = 0.316 x_3$, the reaction (32) becomes

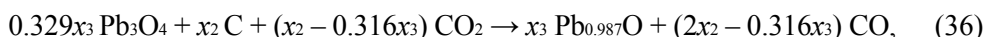


(v) For $x_2 < 0.158 x_3$, from (32) follows



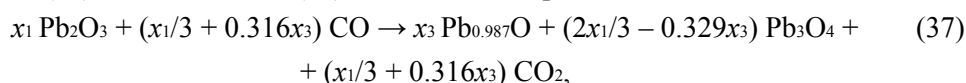
where x_2 and x_3 are arbitrary real numbers.

(vi) For $x_2 > 0.316 x_3$, from (32) follows



where x_2 and x_3 are arbitrary real numbers.

(vii) For $x_2 = 0$, from (28) one obtains this particular reaction

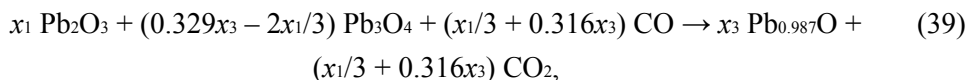


where x_1 and x_3 are arbitrary real numbers. From (37) follows these inequalities $x_1/3 + 0.316x_3 > 0$ and $2x_1/3 - 0.329x_3 > 0$. From this system of inequalities one obtains

$$-x_1/0.048 < x_3 < 2x_1/0.987, \quad (38)$$

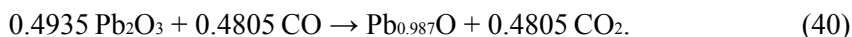
where x_1 and x_3 are arbitrary real numbers. The reaction (37) holds if only if holds the relation (38).

(viii) For $x_1 < 0.4935 x_3$, from (37) follows

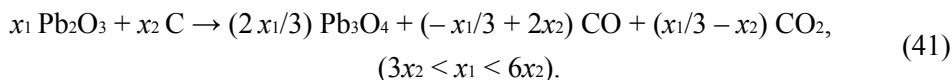


where x_1 and x_3 are arbitrary real numbers.

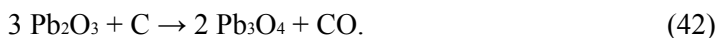
(ix) For $x_1 = 0.4935 x_3$, from (37) follows



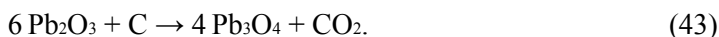
(x) For $x_3 = 0$, from (28) one obtains this particular reaction



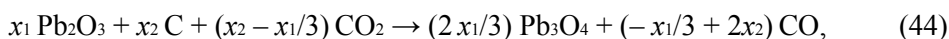
(xi) For $x_1 = 3x_2$, from (41) follows



(xii) For $x_1 = 6x_2$, from (41) one obtains

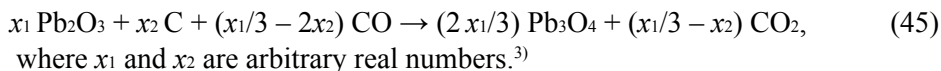


(xiii) For $x_1 < 3x_2$, from (41) follows



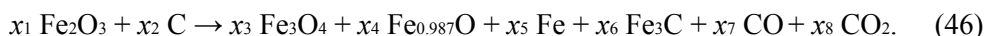
where x_1 and x_2 are arbitrary real numbers.

(xiv) For $x_1 > 6x_2$, from (41) follows



Problem

Now, we shall balance the chemical reaction below



Solution

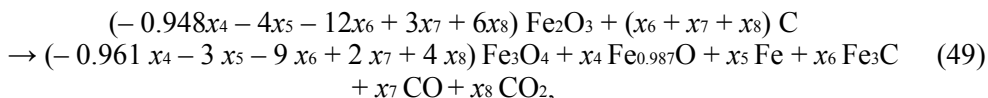
From (46) follows the system

$$\begin{aligned} 2x_1 &= x_3 + 0.987x_4 + x_5 + 3x_6, \\ 3x_1 &= 4x_3 + x_4 + x_7 + 2x_8, \\ x_2 &= x_6 + x_7 + x_8. \end{aligned} \quad (47)$$

The general solution of (47) is

$$\begin{aligned} x_1 &= -0.948x_4 - 4x_5 - 12x_6 + 3x_7 + 6x_8, \\ x_2 &= x_6 + x_7 + x_8, \\ x_3 &= -0.961x_4 - 3x_5 - 9x_6 + 2x_7 + 4x_8, \end{aligned} \quad (48)$$

where x_4, x_5, x_6, x_7 and x_8 are arbitrary real numbers. The Balanced chemical reaction (46) has now the form



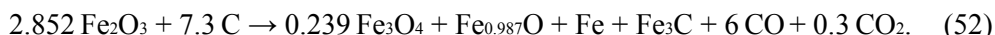
where x_4, x_5, x_6, x_7 and x_8 are arbitrary real numbers. The reaction (49) holds if only if are satisfied the following inequalities

$$x_7 + 2x_8 > 0.4805x_4 + 1.5x_5 + 4.5x_6 \quad (50)$$

and

$$0 < x_7 < 0.4805x_4 + 1.5x_5 + 4.5x_6, \quad (51)$$

where x_4, x_5 and x_6 are arbitrary real numbers. For instance, if $x_4 = x_5 = x_6 = 1$, then from (51) one obtains $x_7 < 6.4805$. Let it be $x_7 = 6$. Then from (50) follows $x_8 > 0.24025$, i.e., $x_8 = 0.3$. Now, the reaction (49) will have this particular form



Discussion

Well-known reactions with unique coefficients do not generate challenge for their future study, because right now they are balancing by a computer very easy. Generally speaking, now it is a "piece of cake". In chemistry, the study of impossible chemical reactions is completely neglected, because they do not have any applicable meaning. Only the class of *continuum chemical reactions* attracts attention for research. That

was our main reason why we considered only special chemical reactions which have non-unique coefficients. This class of chemical reactions is not enough studied in the scientific literature.

What we did? For every considered chemical reaction we determined its general solution. The coefficients of the general solution of every reaction represent the generators which produce an infinite number of solutions. Since they are positive real numbers, from the obtained systems of inequality we determined the necessary and sufficient conditions for every reaction for which it is possible. It is a completely new issue, which until now in chemistry was not considered as an important matter for balancing chemical reactions. Why? Reply on this question is very easy. To date chemists balanced only elementary particular reactions and they did not take into account reaction necessary and sufficient conditions as important factors for its balance possibility. They did not pay attention for general cases and precise criteria for balancing chemical reaction too. In this article we made a new algebra, where are determined very accurately algebraic criteria, for which the particular reaction holds, on such a way, that necessary and sufficient conditions shape the reaction form.

In any way, the *continuum chemical reactions* have an evolutionary property, which directly depends of relations among reaction coefficients. These special reactions are very sensitively connected with the necessary and sufficient conditions for which reactions hold. They are vital parameters for reaction form. These conditions represent an interval where chemical reaction is possible. A change of these conditions, withdraw a change of reaction form. By the necessary and sufficient conditions of reaction one can modify reaction form. It is explicitly shown by the examples above. Roughly speaking, determination of reaction generators without precisely determined necessary and sufficient conditions for which that reaction holds, it does not mean that reaction is balanced.

Conclusion

Necessary and sufficient conditions for which some reaction holds are essential parameters for reaction form. These conditions show relations among coefficients. Actually, these conditions determine the reaction interval of its possibility. Reaction varieties are possible only by modification of its necessary and sufficient conditions.

By determination of reaction generators, actually is determined its general form. For that case, reaction is possible for infinite coefficient sets, which do not give its interval of possibility. In order to avoid that awkward situation, one can recommend that always must be determined reaction necessary and sufficient conditions for which it holds. Only on that way, in the sense of the new algebra developed in this paper we shall have a completely balanced reaction with accurately determined its necessary and sufficient conditions.

NOTES

1. For the reaction (1), the minimal values of its coefficients were determined by Risteski (2009).
2. The reaction (8) was not new Jensen's chemical reaction. Actually, it represents only a slight modification of the well-known Willard's (1912) reaction. Also, Weltin (1994) studied the above reaction (8), but unfortunately he did not offer its solution. By using of a new singular matrix method Risteski (2009) determined its minimal coefficients. By application of the material balance technique a general solution and two particular solutions of (8) were obtained by Petkova et al. (2010).
3. Atanassova (2009) has given a particular technique for balancing elementary chemical reactions, which is useful only for reactions that possess unique coefficients, but it is not an *alternative method* as the author says. For instance, next example we shall use as a counterexample, which shows powerlessness of that particular technique for reaction with non-unique coefficients.

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✉ Dr. Ice B. Risteski,
2 Milepost Place # 606, Toronto, Ontario,
Canada M4H 1C7
E-mail: ice@scientist.com