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Mathematical model for some chemical Redox reactions

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Abstract

Algebraic hyperstructures have many applications in various sciences. The main purpose of this paper is to provide a new application of weak hyperstructures in chemistry. The motivation for the study of hyperstructures comes from chemical reactions. By hyperstructures theory, we provide mathematical models for chemical reactions. We study chemical hyperstructures of standard reduction potentials for consecutive oxidation states of elements of $Cm; Er; Pm; Mg; Tm; Au$ and Cf.

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1 Introduction

Algebraic hyperstructures represent a field of algebra of significant attraction and productive of many significant results in other science. There are many topics about hyperstructures, which can be in depth analyzed and there also are open problems and new connections to other fields that can be explored more in the future. The concept of hypergroup was introduced in 1934 by a French mathematician F. Marty [7], at the 8^{th} Congress of Scandinavian Mathematicians. He published some notes on hypergroups, using them in different contexts: algebraic functions, rational fractions, non-commutative groups. In [1, 10, 11, 12, 13], several of the numerous applications of hyperstructures are presented, especially those that were found and studied in the last fifteen years. There are applications to the following subjects: geometry, hypergraphs, binary relations, lattices, fuzzy sets and rough sets, automata, cryptography, median algebra, relation algebras, combinatorics, codes, artificial intelligence, and probabilities. Also, we can see some other recent applications of hyperstructures in chemistry and physics.

Motivation for the study of hyperstructures comes from chemical reactions. This study focused on the relationship between algebraic hyperstructures and chemistry. The goal of this paper is to

help mathematics by offering suggestions about how algebraic hyperstructures and chemistry can be coordinated better in curriculum. We study chemical hyperstructures of standard reduction potentials for consecutive oxidation states of elements of Cm, Er, Pm, Mg, Tm, Au and Cf.

2 Electrode potentials

Redox reactions are reactions in which one species is reduced, and another is oxidized. Therefore the oxidation state of the species involved must change. These reactions are essential for many applications, including energy storage devices (batteries), photographic processing, and energy production and utilization in living systems, including humans. In reduction, an atom gains an electron and therefore reduces its oxidation number, and in the oxidation, an atom loses an electron and therefore increases its oxidation number [5, 6, 8, 9]. For example, consider the redox reaction shown below:

$$Fe^{2+} + Ce^{4+} \longrightarrow Fe^{3+} + Ce^{3+}.$$

In this process, the Fe^{2+} ion is oxidized, but no oxygen is involved in this reaction. The Ce^{4+}, which is reduced, acts as the oxidizing agent. So, oxidation reactions need not involve oxygen. This redox reaction is actually the sum of two separate half-reactions (a reduction half-reaction and an oxidation half-reaction).

$$Fe^{2+} \longrightarrow Fe^{3+} + e,$$
$$Ce^{4+} + e \longrightarrow Ce^{3+}.$$

The accepted convention is to give the potentials of half reactions as reduction process. The E values corresponding to reduction half reactions with all solutes at 1 mol and all gases at 1 atom are called standard reduction potentials. Each half-reaction has a standard reduction potential E^0, which is equal to the potential difference at equilibrium under standard conditions of an electrochemical cell in which the cathode reaction is the half-reaction considered, and the anode is a standard hydrogen electrode (SHE. The accepted convention is to give the potentials of half reactions as reduction process. The E^0 values corresponding to reduction half reactions with all solutes at 1 mol and all gases at 1 atm are called standard reduction potentials. In an electrochemical cell, the over all cell EMF, E^0 cell, is calculated to be the sum of the potentials of the two half reactions. Furthermore, if the reaction occurs under reversible conditions, the EMF can be related to the free energy change by the equation

$$\Delta G^0 = -nFE^0,$$

where ΔG^0 is the free energy change, n is the number of equivalents oxidized or reduced, and F is the the Faraday constant.
Davvaz et al. [2, 3], considered redox reactions Ag, Cu, Am and Au. They consider the potential of the cell by $E_{cell} = E_{cathode} - E_{anode}$. When the potential of a redox reaction E_{cell} is positive, this reaction will be spontaneous. In this way, we can see that a redox reaction has more than potential numbers. Then, we can not trust the results obtained by the Davvaz. et al. For example, consider the redox reaction:

$$Mn + Mn^3 \to Mn^{2+} + Mn^{6+}.$$

We consider two half-reactions for this reaction:

(1) $Mn^{3+} + e \longrightarrow Mn^{2+}$,

(2) $Mn \longrightarrow Mn^{6+} + 6e$,

$$\begin{cases} Mn^{3+} + 2H_2o & \longrightarrow Mno_2 + 4H^+ + e & E^0 = -.95 \\ Mno_2 + 4H^+ + 2e & \longrightarrow Mno^{2+} + 2H_2o & E^0 = 1.23 \end{cases}$$

$$E_{cathode} = .28.$$

$$\begin{cases} Mn & \longrightarrow Mno^{2+} + 2e & E^0 = 1.18 \\ Mno_4^{-1} + e & \longrightarrow Mno_4^{2-} & E^0 = .564 \\ Mno^{2+} + 4H_2o & \rightarrow Mno_4^- + 8H^+ + 5e & E^0 = -1.51 \end{cases}$$

$$E_{anode} = -.234.$$

Hence, $E_{cell} = .28 - (-234) = .514$.
Also, we can obtain the potential of this cell as follows:

$$\begin{cases} Mn^{3+} + 2H_2o & \longrightarrow Mno_2 + 4H^+ + e & E^0 = -.95 \\ Mno_2 + 2H_2o & \longrightarrow Mno_4^- + 4H^+ + 3e & E^0 = -1.695 \\ Mno_4^- + 8H^+ + 5e & \longrightarrow Mn^{2+} + 4H_2o & E^0 = 1.51 \end{cases}$$

$$E_{cathode} = -1.135.$$

$$\begin{cases} Mn^{2+} + 2e & \longrightarrow Mn & E^0 = -1.18 \\ Mno_2 + 4H^+ + 2e & \longrightarrow Mn^{2+} + 2H_2o & E^0 = 1.23 \\ Mno_4^- + 4H^+ + 3e & \longrightarrow Mno_2 + 2H_2o & E^0 = 1.695 \\ Mno_4^{2-} & \longrightarrow Mno_4^- + e & E = -.564 \end{cases}$$

$$E_{anode} = 1.18.$$

Hence, $E_{cell} = -1.135 - 1.18 = -2.315$. Thus, this reaction has two different potential. This implies that when we use this formula the results are not trusty.

Now, we calculate the potential of a redox reaction by another way. By this way, potential number of a redox reaction is unique. For example, we consider two half reactions:

(1) $Mn^{3+} + e \rightarrow Mn^{2+} + e$,

(2) $Mn \rightarrow Mn^{6+} + 6e$.

$$\begin{cases} Mn^{3+} + 2H_2o & \longrightarrow Mno_2 + 4H^+ + e & E^0 = -.95 \\ Mno_2 + 2H_2o & \longrightarrow Mno_4^- + 4H^+ + 3e^- & E^0 = -1.695 \\ Mno_4^- + 8H^+ + 5e & \rightarrow Mn^{2+} + 4H_2o & E^0 = 1.51 \end{cases}$$

$$E_1 = \frac{(-.95) \times 1 + (-1.695) \times 3 + (1.51) \times 5}{1} = 1.51.$$

$$\begin{cases} Mn & \longrightarrow Mn^{2+} + 2e & E^0 = 1.18 \\ Mn^{2+} + 2H_2o & \longrightarrow Mno_2 + 4H^+ + 2e^- & E^0 = -1.23 \\ Mno_2 + 2H_2o + 5e & \longrightarrow Mno_4^- + 4H^+ + 3e & E^0 = -1.695 \\ Mno_4^- + e & \longrightarrow Mno_4^{2-} & E^0 = .564 \end{cases}$$

$$E_2 = \frac{2(1.18) + 2(-1.23) + 3(-1.695) + .564}{6} = -.77.$$

$$E_{cell} = \frac{1(1.51) + 6(-.77)}{5} = -.622.$$

Also, we can the potential of these cells by a different way as follows:

$$\begin{cases} Mn^{3+} + 2H_2o \longrightarrow Mno_2 + 4H^+ + e & E^0 = -.95 \\ Mno_2 + 4H^+ + 2e \longrightarrow Mno^{2+} + 2H_2o & E^0 = 1.23 \end{cases}$$

$$E_1 = \frac{1(-.95) + 3(-1.695) + 3(1.23)}{6} = 1.51.$$

$$\begin{cases} Mn \longrightarrow Mn^{2+} + 2e & E^0 = 1.18 \\ Mno_4^- + e \longrightarrow Mno_4^{2-} & E^0 = .564 \\ Mn^{2+} + 4H_2o \longrightarrow Mno_4^- + 8H^+ + 5e & E^0 = -1.51 \end{cases}$$

$$E_2 = \frac{2(1.18) + 5(-1.51) + .564}{6} = -.77.$$

$$E_{cell} = \frac{1(1.51) + 6(-.77)}{5} = -.622.$$

Hence, we obtain unique potential number.

3 Algebraic hyperstructure

Algebraic hyperstructures are a suitable generalization of classical algebraic structures. In a classical algebraic structure, the composition of two elements is an element, while in an algebraic hyperstructure, the composition of two elements is a set. More exactly, if H be a nonempty set and $P^*(H)$ the set of all nonempty subsets of H, then we consider $\circ : H \times H \longrightarrow P^*(H)$ as a hyperoperation and the couple $(H, \circ)$ is called *hypergroupoid*. Also, for two nonempty subsets A and B of H and $x \in H$, we define

$$A \circ B = \bigcup_{a \in A,\ b \in B} a \circ b, \quad A \circ x = A \circ \{x\}, \quad x \circ B = \{x\} \circ B.$$

H_v-structures were introduced by Vougiouklis at the Fourth AHA congress (1990)[13]. The concept of an H_v-structure constitutes a generalization of the well-known algebraic hyperstructures. Actually, axioms concerning hyperstructures, such as the associative law, the distributive law, and so on are replaced by their corresponding weak axioms.

Definition 3.1. [4] *Let $(H, \circ)$ be a hypergroupoid. Then, H is called an H_v-semigroup if*

$$\forall x, y, z \in H \quad (x \circ y) \circ z \cap x \circ (y \circ z) \neq \emptyset.$$

An H_v-semigroup H is called an H_v-group if for every $x \in H$, we have

$$x \circ H = x \circ H = H.$$

Definition 3.2. [4] *Let $(H_1, \circ)$ and $(H_2, *)$ be two H_v-groups and $\varphi : H_1 \longrightarrow H_2$ be a map. Then, φ is called a homomorphism, when for every $x, y \in H_1$,*

$$\varphi(x \circ y) = \varphi(x) * \varphi(y).$$

A homomorphism φ is called isomorphism when one to one and onto.

4 Redox reaction of Yb

Ytterbium is a chemical element with the symbol Yb and atomic number 70. It have three oxidation states of 0, 2, 3. All possible products for spontaneous reactions as follows:

$$Yb + Yb^{2+} \longrightarrow Yb + Yb^{3+}, \quad \begin{cases} Yb \longrightarrow Yb^{3+} + 3e, & E^0 = 2.19 \\ Yb^{2+} + 2e \longrightarrow Yb, & E^0 = -2.76 \end{cases}$$

$$E_{cell} = \frac{3(2.19) + 2(-2.76)}{1} = 1.05.$$

$$Ybr + Yb^{3+} \longrightarrow Yb + Yb^{2+}, \quad \begin{cases} Yb \longrightarrow Yb^{2+} + 2e, & E^0 = 2.76 \\ Yb^{3+} + 3e \longrightarrow Yb, & E^0 = -2.19 \end{cases}$$

$$E_{cell} = \frac{3(-2.19) + 2(2.76)}{1} = -1.05.$$

$$Yb + Yb^{3+} \longrightarrow Yb^{2+} + Ybr^{2+}, \quad \begin{cases} Yb \longrightarrow Yb^{2+} + 2e, & E^0 = 2.76 \\ Yb^{3+} + e \longrightarrow Yb^{2+} & E^0 = -1.05 \end{cases}$$

$$E_{cell} = \frac{(-1.05) + 2(2.76)}{1} = 4.47.$$

$$Yb + Yb^{3+} \longrightarrow Yb^{2+} + Yb^{3+}, \quad \begin{cases} Yb \longrightarrow Yb^{3+} + 3e, & E^0 = 2.19 \\ Yb^{3+} + e \longrightarrow Yb^{2+} & E^0 = -1.05 \end{cases}$$

$$E_{cell} = \frac{(-1.05) + 3(2.19)}{2} = 2.76.$$

$$Yb^{2+} + Yb^{2+} \longrightarrow Yb + Yb^{3+}, \quad \begin{cases} Yb^{2+} \longrightarrow Yb^{3+} + e, & E^0 = 1.05 \\ Yb^{2+} + 2e \longrightarrow Yb & E^0 = -2.76 \end{cases}$$

$$E_{cell} = \frac{2(-2.76) + (1.05)}{1} = -4.47.$$

$$Yb^{2+} + Yb^{3+} \longrightarrow Yb + Yb^{3+}, \quad \begin{cases} Yb^{2+} \longrightarrow Yb^{3+} + e, & E^0 = 2.19 \\ Yb^{3+} + 3e \longrightarrow Yb & E^0 = -1.05 \end{cases}$$

$$E_{cell} = -2.76.$$

Therefore, all possible products in reactions between oxidation states of Yb which can be produced spontaneously are listed in Table 1.

Table 1: Redox Reactions Yb

$\oplus$	Yb	Yb^{2+}	Yb^{3+}
Yb	Yb	Yb, Yb^{3+}	Yb^{2+}, Yb^{3+}
Yb^{2+}	Yb, Yb^{3+}	Yb^{2+}	Yb^{2+}, Yb^{3+}
Yb^{3+}	Yb^{2+}, Yb^{3+}	Yb^{2+}, Yb^{3+}	Yb^{3+}

5 Redox reaction of Sm

Samarium is a chemical element with symbol Sm and atomic number 62. It is a moderately hard silvery metal that slowly oxidizes in air. It have three oxidation states of 0, 2, 3. All possible products for spontaneous reactions as follows:

$$Sm^{2+} + Sm \longrightarrow Sm + Sm^{3+}, \quad \begin{cases} Sm \longrightarrow Sm^{3+} + 3e, & E^0 = 2.304 \\ Sm^{2+} + 2e \longrightarrow sm & E^0 = -2.68 \end{cases}$$

$$E_{cell} = \frac{2(-2.68) + 3(2.304}{2} = -1.552.$$

$$Sm + Sm^{3+} \longrightarrow Sm^{2+} + Sm^{2+}, \quad \begin{cases} Sm \longrightarrow Sm^{2+} + 2e, & E^0 = 2.28 \\ Sm^{2+} + 2e \longrightarrow sm & E^0 = -1.55 \end{cases}$$

$$E_{cell} = \frac{(-1.55) + 2(2.68}{1} = 3.81.$$

$$Sm + Sm^{3+} \longrightarrow Sm^{2+} + Sm^{3+}, \quad \begin{cases} Sm \longrightarrow Sm^{3+} + 3e, & E^0 = 2.304 \\ Sm^{3+} + e \longrightarrow sm^{2+} & E^0 = -1.55 \end{cases}$$

$$E_{cell} = \frac{(-1.55) + 3(2.304)}{2} = 2.681.$$

$$Sm^{2+} + Sm^{2+} \longrightarrow Sm + Sm^{3+}, \quad \begin{cases} Sm^{2+} \longrightarrow Sm^{3+} + e, & E^0 = 1.55 \\ Sm^{2+} + 2e \longrightarrow sm & E^0 = -2.68 \end{cases}$$

$$E_{cell} = \frac{2(-2.68) + (1.55)}{1} = -3.81.$$

Therefore, all possible combinations for different oxidation states of Sm which can be produced without energy are presented in Table 2.

Table 2: Redox Reactions Sm

$\oplus$	Sm	Sm^{2+}	Sm^{3+}
Sm	Sm	Sm, Sm^{3+}	Sm^{2+}, Sm^{3+}
Sm^{2+}	Sm, Sm^{3+}	Sm^{2+}	Sm^{2+}, Sm^{3+}
Sm^{3+}	Sm^{2+}, Sm^{3+}	Sm^{2+}, Sm^{3+}	Sm^{3+}

6 Redox reaction of Sr

Strontium is the chemical element with the symbol Sr and atomic number 38. It have three oxidation states of 0, 1, 2.

$$Sr + Sr^{+} \longrightarrow Sr + Sm^{2+}, \quad \begin{cases} Sr \longrightarrow Sr^{2+} + 2e, & E^0 = 2.889 \\ Sr^{+} + e \longrightarrow sr & E^0 = -4.1 \end{cases}$$

$$E_{cell} = \frac{(-4.1) + 2(2.899}{1} = 1.698.$$

$$Sr + Sr^{2+} \longrightarrow Sr + Sm^{+}, \quad \begin{cases} Sr \longrightarrow Sr^{+} + e, & E^0 = -4.1 \\ Sr^{2+} + 2e \longrightarrow sr & E^0 = -2.899 \end{cases}$$

$$E_{cell} = \frac{2(-2.899) + 4.1}{1} = -1.698.$$

Therefore, the products in reactions between oxidation states of Sr which can be produced spontaneously are listed in Table 3.

Table 3: Redox Reactions Sr

$\oplus$	Sr	Sr^{+}	Sr^{2+}
Sr	Sr	Sr, Sr^{2+}	Sr^{+}, Sr^{2+}
Sr^{+}	Sr, Sr^{2+}	Sr^{+}	Sr^{+}, Sm^{2+}
Sr^{2+}	Sr^{+}, Sm^{2+}	Sr^{+}, Sm^{2+}	Sm^{2+}

7 Redox reaction of Ca

The chemical element Calcium (Ca), atomic number 20, is the fifth element and the third most abundant metal in the earth's crust. It have three oxidation states of 0,1, 2.

$$Ca + Ca^{+} \longrightarrow Ca + Ca^{2+}, \quad \begin{cases} Ca \longrightarrow Ca^{2+} + 2e, & E^0 = 2.868 \\ Ca + e \longrightarrow Ca & E^0 = -3.8 \end{cases}$$

$$E_{cell} = \frac{(-3.8) + 2(2.828}{1} = 1.936.$$

$$Ca + Ca^{+} \longrightarrow Ca + Ca^{2+}, \quad \begin{cases} Ca \longrightarrow Ca^{2+} + 2e, & E^0 = 2.868 \\ Ca + e \longrightarrow Ca & E^0 = -3.8 \end{cases}$$

$$E_{cell} = \frac{(-3.8) + 2(2.828}{1} = -1.936.$$

$$Ca + Ca^{2+} \longrightarrow Ca^{+} + Ca^{+}, \quad \begin{cases} Ca \longrightarrow Ca^{2+} + 2e, \\ Ca^{2+} + e \longrightarrow Ca^{+} \end{cases}$$

$$E_{cell} = -3.8.$$

All combinational probability for redox reaction Ca to do without energy can be displayed as follows:

Table 4: Redox Reactions Ca

$\oplus$	Ca	Ca^{+}	Ca^{2+}
Ca	Ca	Ca, Ca^{2+}	Ca^{+}, Ca^{2+}
Ca^{+}	Ca, Ca^{2+}	Ca^{+}	Ca^{+}, Ca^{2+}
Ca^{2+}	Ca^{+}, Ca^{2+}	Ca^{+}, Ca^{2+}	Ca^{2+}

8 Conclusion

Mathematical chemistry is the area of research engaged in novel applications of mathematics to chemistry. Chemical reactions are examples of the phenomena when the composition of two or more elements is a non-empty set of elements. This study focused on the relationship between algebraic hyperstructures and chemistry. The goal of this paper is to help mathematics by offering suggestions about how algebraic hyperstructures and chemistry can be coordinated better in the curriculum. By hyperstructures theory, we provide mathematical models for chemical reactions. We study chemical hyperstructures of standard reduction potentials for consecutive oxidation states of elements of Cm, Er, Pm, Mg,Tm, Au and Cf. Some of the induced H_v-groups by redox reactions are isomorphic and in future work, we consider chemical reasons for this. Although the obtained results are interesting, more investigation on the application of this study in chemistry is required and should be considered in the future work.

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