

CHEMICAL HYPERSTRUCTURES OF CHEMICAL REACTIONS FOR IRON AND INDIUM

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ABSTRACT. In this paper, we investigate chemical hyperstructures of chemical reactions for iron and indium using hyperstructure theory.

1. Introduction

F. Marty [5] was the first to introduce the theory of algebraic hyperstructures that is generalization of the concept of algebraic structures in 1934. Corsini [1], Corsini and Leoreanu [2] et al. studied for the connection between hyperstructures and binary relations. Also we can know that Vougiouklis [6] studied the class of H_v -groups and their several properties. B. Davvaz, A. D. Nezhad and A. Benvidi especially showed ternary algebraic hyperstructures in chain reactions and chemical hyperalgebra in dismutation reactions [3, 4]. In 2012[4], they had chemical hyperstructures for a set of tin and a set of indium.

In this paper, we study chemical hyperstructures of standard reduction potentials for three consecutive oxidation states of elements of iron and indium. The chemical hyperstructure of the set of tin [4] and the set of iron (Theorem 3.2) are equal. But, for the case of the set of indium ions, we have obtained a different hyperoperation table (Theorem 3.4) of B. Davvaz, A. D. Nezhad and A. Benvidi's result([4], p. 60).

2. Algebraic hyperstructures

Let H be a non-empty set and $\cdot : H \times H \longrightarrow \wp^*(H)$ be a function, where $\wp^*(H)$ is the set of all non-empty subsets of H . Then the function \cdot is called a *hyperoperation* on H and the couple (H, \cdot) is called a *hypergroupoid*. For two

Received March 28, 2014; Accepted April 16, 2014.

2010 Mathematics Subject Classification: Primary 20N20.

Key words and phrases: hyperstructure, hypergroup, H_v -group, oxidation-reduction reaction, disproportionation reaction.

subsets A, B of H , we define $A \cdot B = \cup_{a \in A, b \in B} a \cdot b$, and for a singleton $\{a\}$ we denote $\{a\} \cdot B = a \cdot B$ and $B \cdot \{a\} = B \cdot a$.

The hypergroupoid (H, \cdot) is called a *semihypergroup* if

$$x \cdot (y \cdot z) = (x \cdot y) \cdot z, \text{ for all } x, y, z \in H.$$

The hypergroupoid (H, \cdot) is called an H_v -*semigroup* if

$$x \cdot (y \cdot z) \cap (x \cdot y) \cdot z \neq \emptyset, \text{ for all } x, y, z \in H.$$

The hypergroupoid (H, \cdot) is called a *quasihypergroup* if

$$x \cdot H = H \cdot x = H, \text{ for all } x \in H.$$

The hyperoperation (\cdot) is called *commutative* if

$$x \cdot y = y \cdot x, \text{ for all } x, y \in H.$$

The hypergroupoid (H, \cdot) is called a *hypergroup* if it is a semihypergroup and a quasihypergroup.

The hypergroupoid (H, \cdot) is called an H_v -*group* if it is an H_v -semigroup and a quasihypergroup.

The hypergroupoid (H, \cdot) is called a *commutative hypergroup* if it is a hypergroup with a commutative hyperoperation (\cdot) .

The hypergroupoid (H, \cdot) is called a *commutative H_v -group* if it is an H_v -group with a commutative hyperoperation (\cdot) .

3. Chemical hyperstructures of chemical reactions for iron and indium

Most of elements have oxidation states of positive, negative, and zero value; in addition, most of transition metals have two positive oxidation states and some have more. Reactions in which electrons are exchanged are referred to as oxidation-reduction reactions or redox reactions. This reaction are involved in the synthesis of sodium chloride from the reaction of elemental sodium and chlorine and metal corrosion reaction, and providing energy for cells to carry out daily life processes etc.

For redox reactions that occur in acidic and/or basic solutions, it is useful to separate the reaction into two half reactions: one involving oxidation and the other involving reduction. Electrochemistry is defined as the study of the interchange of chemical and electrical energy. In thermodynamics, spontaneous chemical reaction generates electricity and the opposite process, the use of electricity occurs chemical change.

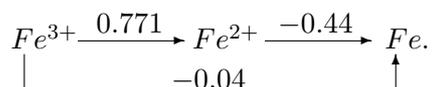
The accepted convention is to give the potentials of half reactions as reduction process. The E° values corresponding to reduction half reactions with all solutes at 1 mol and all gases at 1 atm are called *standard reduction potentials*. In an electrochemical cell, the over all cell EMF, E° cell, is calculated to be the sum of the potentials of the two half reactions. And also if the reaction occurs under reversible conditions, the EMF can be related to the free energy change by the equation

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

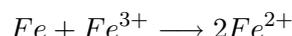
where ΔG° is the free energy change, n is the number of equivalents oxidized or reduced and F is the the Faraday constant ($9.64853 \times 10^4 C/mol$).

Through the Latimer diagrams of all elements, we selected iron (Fe) and indium (In) that were recorded three consecutive standard reduction potentials in acidic solutions.

In [7], we obtain

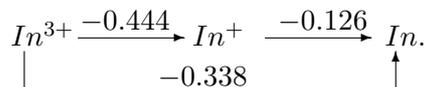


an element iron(Fe) in the oxidation states 0 and 4+ can comproportionate to the state 2+. Therefore, the comproportionation reaction

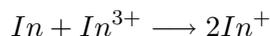


is spontaneous since EMF(0.77 + 0.44) is positive.

In [8], we obtain



But the comproportionation reaction

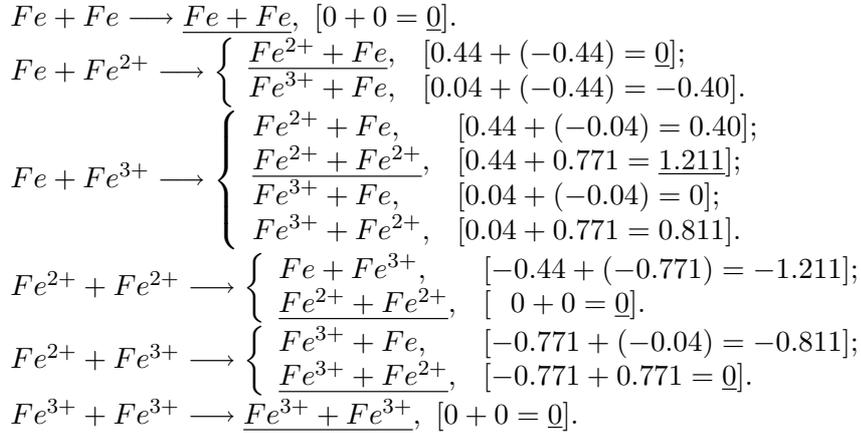


is not spontaneous since EMF($-0.444 + 0.126$) is negative.

The products from the comproportionation of the two elements are different. Therefore, we used a mathematical operation to find the difference between the iron and the indium in the Latimer diagrams.

DEFINITION 3.1. Let G be a set of two or more chemical species and a hyperoperation \oplus on G is defined as follows; for all $x, y \in G$, $x \oplus y$ is defined the *major product*, that is, it is selected from the largest combination among all spontaneous redox reactions.

The following reactions are all possible redox combinations for the set $\{Fe, Fe^{2+}, Fe^{3+}\}$.



The underline $\underline{\quad}$ is the major product. Then we obtain the following hyperoperation table for the set $\{Fe, Fe^{2+}, Fe^{3+}\}$:

\oplus	Fe	Fe^{2+}	Fe^{3+}
Fe	Fe	Fe, Fe^{2+}	Fe^{2+}
Fe^{2+}	Fe, Fe^{2+}	Fe^{2+}	Fe^{2+}, Fe^{3+}
Fe^{3+}	Fe^{2+}	Fe^{2+}, Fe^{3+}	Fe^{3+}

In the above table, if we change the name from Fe, Fe^{2+} and Fe^{3+} to a, b and c , respectively, then the following Theorem 3.2 holds.

THEOREM 3.2. *Let $G_{Fe} = \{a, b, c\}$ and \oplus be the hyperoperation on G_{Fe} . Consider the following commutative hyperoperation table:*

\oplus	a	b	c
a	$\{a\}$	$\{a, b\}$	$\{b\}$
b	$\{a, b\}$	$\{b\}$	$\{b, c\}$
c	$\{b\}$	$\{b, c\}$	$\{c\}$

Then the hyperstructure (G_{Fe}, \oplus) is a commutative H_ν -semigroup.

Proof. For all $x, y, z \in G_{Fe}$, we have

$$\begin{cases} [x \oplus (y \oplus z)] \cap [(x \oplus y) \oplus z] = \{a\}, & \text{if } x = a, y = a, z = a; \\ [x \oplus (y \oplus z)] \cap [(x \oplus y) \oplus z] = \{c\}, & \text{if } x = c, y = c, z = c; \\ [x \oplus (y \oplus z)] \cap [(x \oplus y) \oplus z] \ni b, & \text{otherwise.} \end{cases}$$

Thus $[x \oplus (y \oplus z)] \cap [(x \oplus y) \oplus z] \neq \emptyset$ for all $x, y, z \in G_{Fe}$. □

REMARK 3.3. In Theorem 3.2 $c \oplus (a \oplus a) = c \oplus a = \{b\}$ and $(c \oplus a) \oplus a = b \oplus a = \{a, b\}$. Thus $c \oplus (a \oplus a) \neq (c \oplus a) \oplus a$. Hence G_{Fe} is not a semihypergroup.

For the case iron (Fe), we have the same hyperoperation table for the set $\{Sn, Sn^{2+}, Sn^{4+}\}$ of tin (Sn) in ([4], p. 58). But, for the case indium (In), we have a different hyperoperation table for the set $\{In, In^+, In^{3+}\}$ of indium (In) in ([4], p. 60).

The following are all possible redox combinations for the set $\{In, In^+, In^{3+}\}$.

$$In + In \longrightarrow \underline{In + In}, [0 + 0 = 0].$$

$$In + In^+ \longrightarrow \begin{cases} \underline{In^+ + In}, [0.126 + (-0.126) = 0]; \\ \underline{In^{3+} + In}, [0.338 + (-0.126) = 0.212]. \end{cases}$$

$$In + In^{3+} \longrightarrow \begin{cases} \underline{In^+ + In}, [0.126 + (-0.338) = -0.212]; \\ \underline{In^+ + In^+}, [0.126 + (-0.444) = -0.318]; \\ \underline{In^{3+} + In}, [0.338 + (-0.338) = 0]; \\ \underline{In^{3+} + In^+}, [0.338 + (-0.444) = -0.106]. \end{cases}$$

$$In^+ + In^+ \longrightarrow \begin{cases} \underline{In + In^{3+}}, [-0.126 + 0.444 = 0.318]; \\ \underline{In^+ + In^+}, [0 + 0 = 0]. \end{cases}$$

$$In^+ + In^{3+} \longrightarrow \begin{cases} \underline{In^{3+} + In}, [0.444 + (-0.338) = 0.106]; \\ \underline{In^{3+} + In^+}, [0.444 + (-0.444) = 0]. \end{cases}$$

$$In^{3+} + In^{3+} \longrightarrow \underline{In^{3+} + In^{3+}}, [0 + 0 = 0].$$

The underline $\underline{\quad}$ is the major product. Then we obtain the following hyperoperation table for the set $\{In, In^+, In^{3+}\}$:

\oplus	In	In^+	In^{3+}
In	In	In, In^{3+}	In, In^{3+}
In^+	In, In^{3+}	In, In^{3+}	In, In^{3+}
In^{3+}	In, In^{3+}	In, In^{3+}	In^{3+}

In the above table, if we change the name from In, In^+ and In^{3+} to a, b and c , respectively, then the following theorem holds.

THEOREM 3.4. *Let $G_{In} = \{a, b, c\}$ and \oplus be the hyperoperation on G_{In} . Consider the following commutative hyperoperation table:*

\oplus	a	b	c
a	$\{a\}$	$\{a, c\}$	$\{a, c\}$
b	$\{a, c\}$	$\{a, c\}$	$\{a, c\}$
c	$\{a, c\}$	$\{a, c\}$	$\{c\}$

Then the hyperstructure (G_{In}, \oplus) is a commutative semihypergroup.

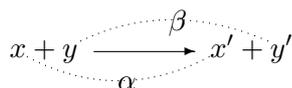
Proof. For all $x, y, z \in G_{In}$, we have

$$x \oplus (y \oplus z) = (x \oplus y) \oplus z = \begin{cases} \{a\}, & \text{if } x = a, y = a, z = a; \\ \{c\}, & \text{if } x = c, y = c, z = c; \\ \{a, c\}, & \text{otherwise.} \end{cases}$$

Thus $x \oplus (y \oplus z) = (x \oplus y) \oplus z$ for all $x, y, z \in G_{In}$. \square

Next we give another chemical hyperoperation.

DEFINITION 3.5. Let G be a set of two or more chemical species and a hyperoperation \oplus' on G is defined as follows; for all $x, y, x', y' \in G$, consider the following all possible combinations for oxidation-reduction reactions



where α and β are potential differences. We define $x \oplus' y$ as follows;

$$x \oplus' y = \begin{cases} \cup_{\alpha+\beta>0} \{x', y'\}, & \text{whenever } x + y \rightarrow x' + y'; \\ \{x, y\}, & \text{otherwise.} \end{cases}$$

THEOREM 3.6. We have the following.

- (1) Let $G_{Fe} = \{a, b, c\}$ and let $a = Fe$, $b = Fe^{2+}$ and $c = Fe^{3+}$. Then we have the following commutative hyperoperation table:

\oplus'	a	b	c
a	$\{a\}$	$\{a, b\}$	$\{a, b, c\}$
b	$\{a, b\}$	$\{b\}$	$\{b, c\}$
c	$\{a, b, c\}$	$\{b, c\}$	$\{c\}$

and the hyperstructure (G_{Fe}, \oplus') is a commutative hypergroup.

- (2) Let $G_{In} = \{a, b, c\}$ and let $a = In$, $b = In^+$ and $c = In^{3+}$. Then we have the following commutative hyperoperation table:

\oplus'	a	b	c
a	$\{a\}$	$\{a, c\}$	$\{a, c\}$
b	$\{a, c\}$	$\{a, c\}$	$\{a, c\}$
c	$\{a, c\}$	$\{a, c\}$	$\{c\}$

and the hyperstructure (G_{In}, \oplus') is a commutative semihypergroup. In this case, both (G_{In}, \oplus) and (G_{In}, \oplus') are the same semihypergroup.

Proof. (1) Using all possible redox combinations (page 322) for the set of iron, we get the hyperoperation tables.

For all $x, y, z \in G_{Fe}$ we have

$$x \oplus' (y \oplus' z) = (x \oplus' y) \oplus' z = \begin{cases} \{a\}, & \text{if } x = a, y = a, z = a; \\ \{b\}, & \text{if } x = b, y = b, z = b; \\ \{c\}, & \text{if } x = c, y = c, z = c; \\ \{a, b\}, \{b, c\} \text{ or } \{a, b, c\}, & \text{otherwise.} \end{cases}$$

Clearly for all $x \in G_{Fe}$ we have $x \oplus' G_{Fe} = G_{Fe} \oplus' x = G_{Fe}$.

(2) Using all possible redox combinations for the set $\{In, In^{2+}, In^{3+}\}$ (page 323), we get the hyperoperation tables. The proof is similar to the proof of Theorem 3.4. \square

Acknowledgement

I thank professor Sang-Cho Chung for his advice on Mathematics.

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