

## CHEMICAL HYPERSTRUCTURES FOR TITANIUM

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ABSTRACT. In this paper, I give chemical hyperstructures of chemical reactions for a set of Titanium( $Ti$ ).

### 1. Introduction

It is very interesting to understand chemical reactions through algebraic hyperstructures. The French mathematician F. Matty [11], who expanded the classical algebraic structure, introduced an algebraic hyperstructure in 1934. P. Corsini, V. Leoreanu, and B. Davvaz [4, 5, 8] *et. al.* also compiled a lot of research results on hyperstructure theory. Also, the study for the class  $H_v$ -groups and their properties was carried out by Vougiouklis [12]. Ternary algebraic hyperstructures in chain reactions and chemical hyperalgebra in redox reactions have been established by B. Davvaz, A. D. Nezhad, and A. Benvidi [6, 7]. S. C. Chung and K. M. Chun [1, 3] reported chemical hyperalgebras for three consecutive oxidation states of elements.

In 2016, B. Davvaz [9] obtained chemical hyperalgebras of Americium(Am), Copper(Cu) and Gold(Au) for four consecutive oxidation states. In this paper, I show results for different chemical hyperalgebras from that of B. Davvaz for Titanium(Ti)

### 2. Hyperalgebraic structures

For a non-empty set  $H$ , a function  $\cdot : H \times H \rightarrow \wp^*(H)$  with the set of all non-empty subsets of  $H$   $\wp^*(H)$  is called a *hyperoperation* on  $H$  and the couple  $(H, \cdot)$  is called a *hypergroupoid*. For two subsets  $A, B$  of  $H$ , we define

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$A \cdot B = \cup_{a \in A, b \in B} a \cdot b$ , 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

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

In this case, the hyperoperation  $(\cdot)$  is called *associative*.

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

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

In this case, the hyperoperation  $(\cdot)$  is called *weakly associative*.

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  $(\cdot)$ .

A non-empty subset  $K$  of a hypergroup (respectively,  $H_v$ -group)  $H$  is called a *subhypergroup* (respectively,  $H_v$ -subgroup) of  $H$  if  $a \cdot K = K \cdot a = K$  for all  $a \in K$ .

Let  $(H_1, \cdot)$  and  $(H_2, *)$  be two  $H_v$ -groups. A map  $f : H_1 \rightarrow H_2$  is called an  $H_v$ -*homomorphism* or *weak homomorphism* if

$$f(x \cdot y) \cap f(x) * f(y) \neq \emptyset \text{ for all } x, y \in H_1.$$

$f$  is called an *inclusion homomorphism* if

$$f(x \cdot y) \subset f(x) * f(y) \text{ for all } x, y \in H_1.$$

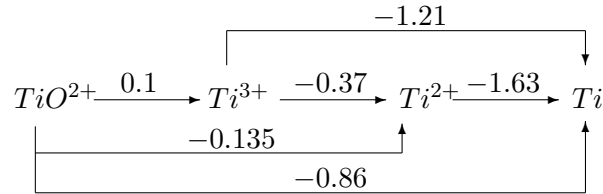
Finally,  $f$  is called a *strong homomorphism* if

$$f(x \cdot y) = f(x) * f(y) \text{ for all } x, y \in H_1.$$

If  $f$  is onto, one to one and strong homomorphism, then it is called an *isomorphism*. In this case,  $H_1$  and  $H_2$  are called *isomorphic* and we write  $H_1 \cong H_2$ .

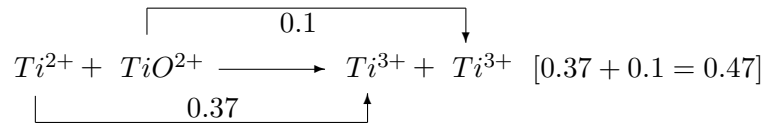
### 3. Chemical hyperstructures of chemical reactions for titanium

There are many kinds of chemical reactions. Any chemical reaction in which the oxidation states of the atoms are changed is an oxidation-reduction (redox reaction). Redox reactions consist of two parts, a reduced half and an oxidized half, that always occur together. Oxidation is the loss of electrons from the reducing agent (which is said to have “been oxidized” in the process). Since electrons carry negative charges, oxidation results in an increase of positive value. Reduction is the gain of electrons by the oxidizing agent. Most transition metals have two positive oxidation states and some have more. Titanium (Ti) has three positive oxidation states of +2, +3, and +4. Among these oxidation states, +2 exists very limitedly. For Titanium [13], we obtain the following.

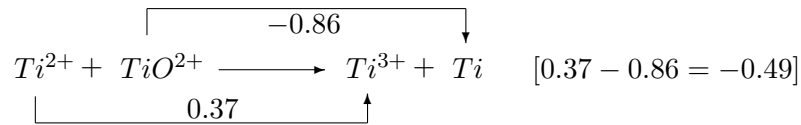


In the above standard reduction potentials, values not given in [13] are calculated by way of the reference [10].

EXAMPLE 3.1. Consider the following case.

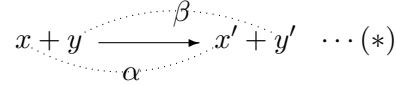


Since the electromotive force ( $E^\circ = 0.47$ ) is positive, that is, the free energy change ( $\Delta G^\circ = -nFE^\circ$ ) is negative, redox reactions under the standard conditions are spontaneous. But for the following case



the electromotive force ( $E^\circ = -0.49$ ) is negative, that is, the free energy change ( $\Delta G^\circ$ ) is positive, therefore redox reactions under the standard conditions are not spontaneous.

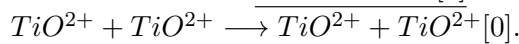
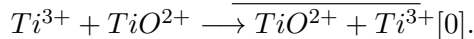
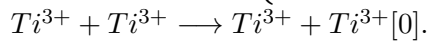
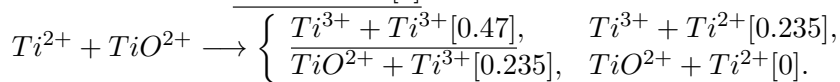
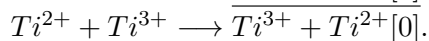
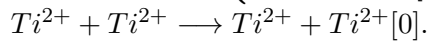
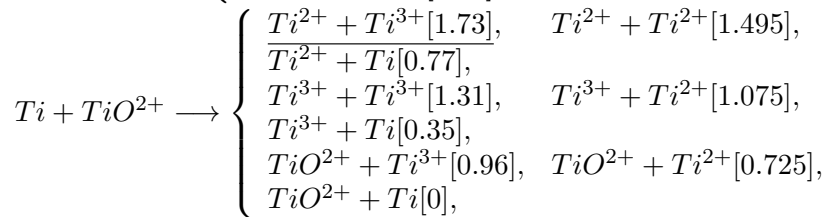
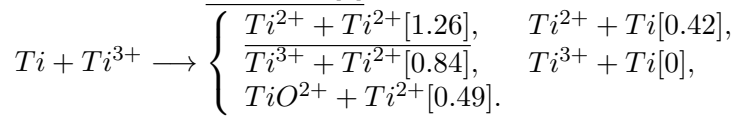
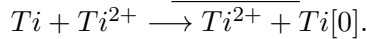
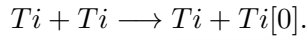
For Titanium elements  $x, y, x', y'$ , consider the following all possible combinations for oxidation-reduction reactions



where  $\alpha$  and  $\beta$  are potential differences. If  $\alpha + \beta > 0$ , then redox reactions under the standard conditions are spontaneous but not for the case  $\alpha + \beta < 0$ .

For a set of two or more chemical species  $G$ , a hyperoperation  $\oplus : G \times G \rightarrow \wp^*(G)$  is defined as follows: for all  $x, y \in G$ ,  $x \oplus y$  is defined as the *major product*, that is, it is chosen from the largest combination among all spontaneous redox reactions.

The following are all possible spontaneous redox combinations for the set  $\{Ti, Ti^{2+}, Ti^{3+}, TiO^{2+}\}$  of Titanium. From now on, we denote  $x + y \rightarrow x' + y'[\gamma]$  instead of  $x + y \rightarrow x' + y'[\alpha + \beta = \gamma]$ , and the underline      is the major product.



Then we obtain the following hyperoperation table [Table 1] for the set of Titanium  $\{Ti, Ti^{2+}, Ti^{3+}, Ti^{4+}(TiO^{2+})\}$ . In [Table 1] the data represents the most stable chemical species that can be present in a thermodynamic method. To determine the thermodynamics of redox reactions, we must first know the

TABLE 1. Redox Reactions Ti.

$\oplus$	$Ti$	$Ti^{2+}$	$Ti^{3+}$	$Ti^{4+}$
$Ti$	$Ti$	$Ti, Ti^{2+}$	$Ti^{2+}$	$Ti^{2+}, Ti^{3+}$
$Ti^{2+}$	$Ti, Ti^{2+}$	$Ti^{2+}$	$Ti^{2+}, Ti^{3+}$	$Ti^{3+}$
$Ti^{3+}$	$Ti^{2+}$	$Ti^{2+}, Ti^{3+}$	$Ti^{3+}$	$Ti^{3+}, Ti^{4+}$
$Ti^{4+}$	$Ti^{2+}, Ti^{3+}$	$Ti^{3+}$	$Ti^{3+}, Ti^{4+}$	$Ti^{4+}$

standard reduction potentials,

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

where  $\Delta G^\circ$  is the free energy change,  $n$  is the number of electrons that is oxidized or reduced and  $F$  is the Faraday constant ( $9.64853 \times 10^4 C/mol$ ).

The hyperstructures of Titanium(Ti) [Table 1] are different from those of Americium(Am), Copper(Cu) and Gold(Au) [9], but the hyperstructures of Titanium(Ti) are isomorphic commutative  $H_v$ -subsemigroups of Vanadium(V) [2, Theorem 3.3].

In the above table, if we change the name from  $Ti, Ti^{2+}, Ti^{3+}$  and  $Ti^{4+}$  to  $a, b, c$  and  $d$ , respectively, then the following theorem holds.

**THEOREM 3.2.** *Let  $G = \{a, b, c, d\}$  be the set of Titanium and  $\oplus$  be the hyperoperation on  $G$ . Consider the following commutative hyperoperation table:*

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

Then we have the following:

- (1) The hyperstructures  $(\{a, b\}, \oplus)$ ,  $(\{b, c\}, \oplus)$  and  $(\{c, d\}, \oplus)$  are commutative subhypergroups of  $G$  and isomorphic.
- (2) The hyperstructures  $(\{a, b, c\}, \oplus)$  and  $(\{b, c, d\}, \oplus)$  are commutative  $H_v$ -subsemigroups of  $G$  and isomorphic.
- (3) The hyperstructure  $(G, \oplus)$  is a commutative  $H_v$ -semigroup.

*Proof.* For all  $x, y, z \in G$ , we show that  $[x \oplus (y \oplus z)] \cap [(x \oplus y) \oplus z] \neq \emptyset$ .

- (1) It is obvious.
- (2) For all  $x, y, z \in \{a, b, c\}$ , we have

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

But clearly it is not a quasihypergroup. Thus  $(\{a, b, c\}, \oplus)$  is a commutative  $H_v$ -semigroup.

Since  $\{a, b, c\}$  and  $\{b, c, d\}$  have the same similar hyperoperation tables, they are isomorphic.

(3) For all  $x, y, z \in \{a, b, c, d\}$ , we have

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

Thus  $(G, \oplus)$  is a commutative  $H_v$ -semigroup. □

REMARK 3.3. The hyperstructure  $(\{a, b, c\}, \oplus)$  is not a semihypergroup since the hyperoperation  $\oplus$  is not associative; for example,  $c \oplus (a \oplus a) = c \oplus a = \{b\}$  and  $(c \oplus a) \oplus a = b \oplus a = \{a, b\}$ . Hence  $c \oplus (a \oplus a) \neq (c \oplus a) \oplus a$ .

Let  $G = \{a, b, c, d\}$  be the set of Titanium and a hyperoperation  $\oplus' : G \times G \rightarrow \wp^*(G)$  is defined as follows:

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

THEOREM 3.4. Let  $G = \{a, b, c, d\}$  be the set of Titanium and  $\oplus'$  be the hyperoperation on  $G$ . Then we have the following:

(1) The hyperstructure  $(G, \oplus')$  has the following commutative hyperoperation table:

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

(2) The hyperstructures  $(\{a, b\}, \oplus')$ ,  $(\{b, c\}, \oplus')$  and  $(\{c, d\}, \oplus')$  are commutative subhypergroups of  $G$  and isomorphic.

(3) The hyperstructure  $(\{b, c, d\}, \oplus')$  is a commutative subhypergroup of  $G$ .

(4) The hyperstructure  $(G, \oplus')$  is a commutative hypergroup.

*Proof.* (1) Using all possible redox reactions(p. 462), we get the hyperoperation table.

(2) It is obvious.

(3) For all  $x, y, z \in \{b, c, d\}$ , we have

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

Thus  $(\{b, c, d\}, \oplus')$  is a commutative hypergroup since it is a quasihypergroup.

(4) It is sufficient to consider all other cases except for the range used in (3). In fact, for all  $x, y, z \in \{a, b, c, d\}$ , we have

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

Thus  $(G, \oplus')$  is a commutative hypergroup since it is a quasihypergroup.  $\square$

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