MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **71** (2014) 323-331

ISSN 0340 - 6253

Chemical Hyperalgebra: Redox Reactions

[a]**Bijan Davvaz**, [a]**Akbar Dehghan Nezad**,
[b]**Mohammad Mazloum–Ardakani**

[a]*Department of Mathematics, Yazd University, Yazd, Iran*
davvaz@yazduni.ac.ir , anezhad@yazduni.ac.ir

[b]*Department of Chemistry, Yazd University, Yazd, Iran*
mazloum@yazduni.ac.ir

(Received June 17, 2012)

Abstract

Algebraic hyperstructure theory has a multiplicity of applications to other disciplines. This paper deals with an outline of applications in chemistry. Indeed, we provide examples of hyperstructures and H_v-structures associated with redox reactions (Ag, Cu, Am and Au).

1 Introduction

The hyperstructures were introduced by Marty when he first defined a hypergroup as a set equipped with an associative and reproductive hyperoperation. The motivating example was the quotient of a group by any, not necessary normal, subgroup. Algebraic hyperstructures represent a natural extension 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, see [1]. In [2], Corsini and Leoreanu presented some of the numerous applications of hyperstructures, 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 algebras, relation algebras; combinatorics; codes; artificial intelligence and probabilities. Moreover, algebraic hyperstructures theory

has a multiplicity of applications to other disciplines, for example see [3–7,9,10]. Another book [8] is devoted especially to the study of hyperring theory. Several kinds of hyperrings are introduced and analyzed. The volume ends with an outline of applications in chemistry and physics, analyzing several special kinds of hyperstructures.

2 Algebraic hyperstructures

Let H be a non-empty set, $\mathcal{P}^*(H)$ be the set of all non-empty subsets of H. A hyperoperation on H is a map $\odot : H \times H \longrightarrow \mathcal{P}^*(H)$ and the couple $(H, \odot)$ is called a hypergrupoid (or hyperstructure). If A and B are non-empty subsets of H, then we denote

$$A \odot B = \bigcup_{a \in A, b \in B} a \odot b,$$

and if $x \in H$, then we denote $A \odot x = A \odot \{x\}$ and $x \odot B = \{x\} \odot B$. A hypergrupoid $(H, \odot)$ is called a semihypergroup if for all x, y, z of H we have $(x \odot y) \odot z = x \odot (y \odot z)$. That is,

$$\bigcup_{u \in x \odot y} u \odot z = \bigcup_{v \in y \odot z} x \odot v.$$

A semihypergroup $(H, \odot)$ is called a hypergroup if for all $x \in H$, $x \odot H = H \odot x = H$. A non-empty subset S of the hypergroup H is called a subhypergroup if $a \odot S = S \odot a = S$ for all $a \in S$. H_v-structures first were introduced by Vougiouklis in Fourth AHA congress [15]. The concept of H_v-structures constitute a generalization of the well-known algebraic hyperstructures (hypergroup, hyperring, hypermodule and so on). Actually some axioms concerning the above hyperstructures such as the associative law, the distributive law and so on are replaced by their corresponding weak axioms. The reader will find in [14] some basic definitions and theorems about the H_v-structures.

Let $(H_1, \odot)$ and $(H_2, \star)$ be two hypergroupoids. A map $f : H_1 \to H_2$, is called

- an inclusion homomorphism if for all x, y of H, we have $f(x \odot y) \subseteq f(x) \star f(y)$;
- a homomorphism if for all x, y of H, we have $f(x \odot y) = f(x) \star f(y)$;
- an isomorphism if it is a one to one and onto homomorphism. In this case, we say H_1 and H_2 are isomorphic and we write $H_1 \cong H_2$.

3 Redox reactions

Redox (reduction-oxidation) reactions include all chemical reactions in which atoms have their oxidation state changed. This can be either a simple redox process, such as the oxidation of carbon to yield carbon dioxide (CO_2) or the reduction of carbon by hydrogen to yield methane (CH_4), or a complex process such as the oxidation of glucose ($C_6H_{12}O_6$) in the human body through a series of complex electron transfer processes. Oxidation is the loss of electrons or an increase in oxidation state, and reduction is the gain of electrons or a decrease in oxidation state by an analyte (molecule, atom or ion). There can not be an oxidation reaction without a reduction reaction happening simultaneously. Therefore the oxidation alone and the reduction alone are each called a half-reaction, because two half-reactions always occur together to form a whole reaction [13].

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). For a redox reaction, the potential of the cell is defined by: $E^0_{cell} = E^0_{cathode} - E^0_{anode}$. If the potential of a redox reaction (E^0_{cell}) is positive, this reaction will spontaneous [13].

For example, consider the redox reaction of Ag^{2+} with Ag:

$$Ag^{2+} + Ag \quad \longrightarrow \quad Ag^{+}.$$

We can write two half-reactions for this reaction:

(1) $Ag^{2+} + e \quad \longrightarrow \quad Ag^{+}$,

(2) $Ag \quad \longrightarrow \quad Ag^{+} + e$.

The E^0 of the first reaction ($E^0_{cathode}$) is 1.98 V (vs. SHE) and the E^0 of the second reaction (E^0_{anode}) is 0.799 V (vs. SHE) [11]. Therefore, in this case, the E^0_{cell} ($E^0_{cathode} - E^0_{anode} = 1.181$) is positive and the above redox reaction between Ag^{2+} and Ag is spontaneous.

Silver (Ag) is a transition metal and has a large number of applications in jewelry, electrical contacts and conductors, catalysis of chemical reactions, disinfectants and microbiocides. Silver plays no known natural biological role in humans and itself is not toxic, but most silver salts are toxic, and some may be carcinogenic. Ag can be in three

oxidation state: Ag (0), Ag (I) and Ag (II). Among Ag (I) and Ag (II), Ag (I) is very well characterized and many simple ionic compounds are known containing Ag^{+}. However, AgF_2 is known which Ag has oxidation state of II in it. AgF_2 is strongly oxidizing and a good fluorimating agent. But Ag (II) is more stable in complex forms. A number of Ag (II) complexes have been obtained by oxidation of Ag (I) salts is aqueous solution in the presences of the ligand. For example, $[Ag\ (pyridine)_4]^{2+}$ and $[Ag\ (bi\ pyridine)_2]^{2+}$ are quite stable. The +1 oxidation state is the best known oxidation state of silver. Ag^{+} salts are generally insoluble in water with the exception of nitrate, fluoride and perchlorate. Most stable Ag (I) complexes have a linear structure [12].

As described above, Ag species with different oxidation state can react with themselves. All possible products for spontaneous reactions are presented in the following table:

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

Table 1. Redox reactions Ag

Copper (Cu) is a ductile metal with very high thermal and electrical conductivity. It is used as a conductor of heat and electricity, a building material, and a constituent of various metal alloys. Cu can be in four oxidation state: Cu (0), Cu (I), Cu (II) and Cu (III). In nature, copper mainly is as $CuFeS_2$, with oxidation state of II for Cu. Also, Cu can be as Cu_2S or Cu_2O with the oxidation state of I. Pure copper is obtained by electrolytic refining using sheets of pure copper as cathode and impure copper as anode. In this process different ions of Cu, Cu (II) or Cu (I), reduced to Cu (0) at cathode. Cu (III) is generally uncommon, however some its complexes are known [12].

The standard reduction potential (E^0) for conversion of each oxidation state to another are: $E^0\ (Cu^{3+}/Cu^{2+})\ =\ 2.4\ V$, $E^0\ (Cu^{2+}/Cu^{+})=\ 0.153\ V$, $E^0\ (Cu^{2+}/Cu)=$ $0.342\ V$ and $E^0\ (Cu^{+}/Cu)=\ 0.521\ V$, where potentials are versus SHE [11]. According to these standard potentials, and similar to example of Ag, the following reactions are spontaneous:

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

(2) $Cu^{3+} + Cu \longrightarrow Cu^{2+} + Cu^{+}$.

Therefore, all possible products in reactions between oxidation states of Cu which can be produced spontaneously are listed in the below table:

$\odot$	Cu	Cu^{+}	Cu^{2+}	Cu^{3+}
Cu	Cu	$Cu,\ Cu^{+}$	$Cu^{2+},\ Cu$	$Cu^{2+},\ Cu^{+}$
Cu^{+}	$Cu,\ Cu^{+}$	Cu^{+}	$Cu^{2+},\ Cu^{+}$	Cu^{2+}
Cu^{2+}	$Cu,\ Cu^{2+}$	$Cu^{2+},\ Cu^{+}$	Cu^{2+}	$Cu^{2+},\ Cu^{3+}$
Cu^{3+}	$Cu^{+},\ Cu^{2+}$	Cu^{2+}	$Cu^{2+},\ Cu^{3+}$	Cu^{3+}

Table 2. Redox reactions Cu

Americium (Am) is a transuranic radioactive chemical element in actinide series. It have four oxidation states of 0, 2, 3 and 4. The standard reduction potential (E^0) for conversion of each oxidation state to another are: $E^0\ (Am^{4+}/Am^{3+})= 2.6\ V$, $E^0\ (Am^{3+}/Am^{2+})= -2.3\ V$, $E^0\ (Am^{3+}/Am)= -2.048\ V$ and $E^0\ (Am^{2+}/Am)= -1.9\ V$, where potentials are versus SHE [11]. Therefore, the following reaction is spontaneous:

$$Am^{4+} + Am^{2+} \longrightarrow Am^{3+}.$$

Therefore, all possible combinations for different oxidation states of Am which can be produced without energy are presented at the following table:

$\otimes$	Am	Am^{2+}	Am^{3+}	Am^{4+}
Am	Am	$Am,\ Am^{2+}$	$Am,\ Am^{3+}$	$Am,\ Am^{4+}$
Am^{2+}	$Am,\ Am^{2+}$	Am^{2+}	$Am^{2+},\ Am^{3+}$	Am^{3+}
Am^{3+}	$Am,\ Am^{3+}$	$Am^{2+},\ Am^{3+}$	Am^{3+}	$Am^{3+},\ Am^{4+}$
Am^{4+}	$Am,\ Am^{4+}$	Am^{3+}	$Am^{3+},\ Am^{4+}$	Am^{4+}

Table 3. Redox reactions Am

Gold (Au) is a dense, soft, shiny, malleable and ductile metal and can be in four oxidation states of Au (0), $Au\ (I)$, $Au\ (II)$ and $Au\ (III)$. $Au\ (III)$ is common for gold compounds and exist as: Au_2O_3, AuF_3, $AuCl_3$, $AuBr_3$ and $Au\ (OH)_3$. $Au\ (I)$ is much less stable in solution and is stabilized in complexes [12].

The standard reduction potential (E^0) for conversion of each oxidation state to another are: $E^0\ (Au^{3+}/Au^{+})= 1.401\ V$, $E^0\ (Au^{3+}/Au)= 1.498\ V$, $E^0\ (Au^{2+}/Au^{+})= 1.8\ V$ and $E^0\ (Au^{+}/Au)= 1.692\ V$, where potentials are versus SHE [11]. According to these

standard potentials, the following reaction is spontaneous:

$$Au^{2+} + Au \longrightarrow Au^{+}.$$

Therefore, the major products in reactions between oxidation states of Au which can be produced spontaneously are listed in below table:

$\uplus$	Au	Au^{+}	Au^{2+}	Au^{3+}
Au	Au	$Au,\ Au^{+}$	Au^{+}	$Au,\ Au^{3+}$
Au^{+}	$Au,\ Au^{+}$	Au^{+}	$Au^{+},\ Au^{2+}$	$Au^{+},\ Au^{3+}$
Au^{2+}	Au^{+}	$Au^{+},\ Au^{2+}$	Au^{2+}	$Au^{2+},\ Au^{3+}$
Au^{3+}	$Au,\ Au^{3+}$	$Au^{+},\ Au^{3+}$	$Au^{2+},\ Au^{3+}$	Au^{3+}

Table 4. Redox reactions Au

4 Some results

4.1 About Table 1

In Table 1, if we rename $Ag^{2+} := a$, $Ag^{+} := b$ and $Ag := c$, then we obtain the following table:

$\oplus$	a	b	c
a	a	$a,\ b$	b
b	$a,\ b$	b	$b,\ c$
c	b	$b,\ c$	c

This table is isomorphic to the first table of dismutation reactions (page 58, [6]). Therefore, $\oplus$ is weak associative. Also, we conclude that $(\{a, b\}, \oplus)$ and $(\{b, c\}, \oplus)$ are hypergroups.

4.2 About Table 2

In Table 2, we rename Cu, Cu^{+}, Cu^{2+} and Cu^{3+} as follows:

$$Cu := a,\ Cu^{+} := b,\ Cu^{2+} := c \text{ and } Cu^{3+} := d.$$

Then, we obtain the following table:

$\odot$	a	b	c	d
a	a	$a,\ b$	$a,\ c$	$b,\ c$
b	$a,\ b$	b	$b,\ c$	c
c	$a,\ c$	$b,\ c$	c	$c,\ d$
d	$b,\ c$	c	$c,\ d$	d

The hyperoperation $\odot$ is weak associative, for instance

$$(a \odot b) \odot d = \{a, b\} \odot d = \{b, c\},$$
$$a \odot (b \odot d) = a \odot c = \{a, c\}.$$

Hence, we have an H_v-semigroup.

The hyperstructures $(\{a, b\}, \odot)$, $(\{a, c\}, \odot)$, $(\{b, c\}, \odot)$ and $(\{c, d\}, \odot)$ are hypergroups.

Let H be a set with three elements. On H, we define the following hyperoperation:

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

It is easy to see that $\star$ is associative and so $(H, \star)$ is a hypergroup. Now, we have

$$(\{a, b, c\}, \odot) \cong (H, \star).$$

Note that $(\{b, c, d\}, \odot)$ is not semihypergroup, because

$$(b \odot c) \odot d = \{b, c\} \odot d = \{c, d\},$$
$$b \odot (c \odot d) = b \odot \{c, d\} = \{b, c\}$$

4.3 About Table 3

In Table 3, we rename Am, Am^{2+}, Am^{3+} and Am^{4+} as follows:

$$Am := x,\ Am^{2+} := y,\ Am^{3+} := z \text{ and } Am^{4+} := t.$$

Then, we obtain the following table:

$\otimes$	x	y	z	t
x	x	$x,\ y$	$x,\ z$	$x,\ t$
y	$x,\ y$	y	$y,\ z$	z
z	$x,\ z$	$y,\ z$	z	$z,\ t$
t	$x,\ t$	z	$z,\ t$	t

Similar to Table 2, we have

$$(\{x, y, z\}, \otimes) \cong (H, \star).$$

Note that $(\{y, z, t\}, \otimes)$ is not semihypergroup, because

$$(y \otimes z) \otimes t = \{y, z\} \otimes t = \{z, t\}$$
$$y \otimes (z \otimes t) = y \otimes \{z, t\} = \{y, z\}.$$

4.4 About Table 4

In Table 4, we rename Au, Cu^+, Au^{2+} and Au^{3+} as follows:

$$Au := a,\ Au^+ := b,\ Au^{2+} := c \text{ and } Au^{3+} := d.$$

Then, we obtain the following table:

$\uplus$	a	b	c	d
a	a	$a,\ b$	b	$a,\ d$
b	$a,\ b$	b	$b,\ c$	$b,\ d$
c	b	$b,\ c$	c	$c,\ d$
d	$a,\ d$	$b,\ d$	$c,\ d$	d

Let us define the following map

$$a \mapsto y$$
$$c \mapsto t$$
$$b \mapsto z$$
$$d \mapsto x.$$

Then, the H_v-semigroups defined in Table 3 and Table 4 are isomorphic.

References

[1] P. Corsini, *Prolegomena of Hypergroup Theory*, Aviani, Udine, 1993.

[2] P. Corsini, V. Leoreanu, *Applications of Hyperstructure Theory*, Kluwer, Dordrecht, 2003.

[3] B. Davvaz, A. Dehghan Nezhad, Chemical examples in hypergroups, *Ratio Mat.* **14** (2003) 71–74.

[4] B. Davvaz, A. Dehghan Nezhad, Dismutation reactions as experimental verifications of ternary algebraic hyperstructures, *MATCH Commun. Math. Comput. Chem.* **68** (2012) 551–559.

[5] B. Davvaz, A. Dehghan Nezhad, A. Benvidi, Chain reactions as experimental examples of ternary algebraic hyperstructures, *MATCH Commun. Math. Comput. Chem.* **65** (2011) 491–499.

[6] B. Davvaz, A. Dehghan Nezhad, A. Benvidi, Chemical hyperalgebra: Dismutation reactions, *MATCH Commun. Math. Comput. Chem.* **67** (2012) 55–63.

[7] B. Davvaz, R. M. Santilli, T. Vougiouklis, Studies of multivalued hyperstructures for the characterization of matter–antimatter systems and their extension, *Algebras Groups and Geometries* **28** (2011) 105–116.

[8] B. Davvaz, V. Leoreanu–Fotea, *Hyperring Theory and Applications*, Academic Press, Palm Harbor, 2007.

[9] A. Delavar Khalafi, B. Davvaz, Algebraic hyperstructures associated to convex analysis and applications, *Filomat* **26** (2012) 55–65.

[10] M. Ghadiri, B. Davvaz, R. Nekouian, H_v–semigroup structure on F_2–offspring of a gene pool, *Int. J. Biomath.* **5** (2012) 1250011 (13 pages).

[11] D. R. Lide (Ed.), *CRC Handbook of Chemistry and Physics*, CRC Press, Boca Raton, 2005.

[12] M. S. Sethi, M. Satake, *Chemistry of Transition Elements*, South Asian, New Delhi, 1988.

[13] D. A. Skoog, D. M. West, F. J. Holler, *Fundamentals of Analytical Chemistry*, Saunders College, Philadelphia, 1988.

[14] T. Vougiouklis, *Hyperstructures and Their Representations*, Hadronic Press, Palm Harbor, 1994.

[15] T. Vougiouklis, *The Fundamental Relation in Hyperrings. The General Hyperfield, Algebraic Hyperstructures and Applications, (Xanthi, 1990)*, World Sci. Publishing, Teaneck, 1991, pp. 203–211.