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Chain Reactions as Experimental Examples of Ternary Algebraic Hyperstructures

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Abstract

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. Algebraic hyperstructure theory has a multiplicity of applications to other disciplines. The main purpose of this paper is to provide examples of ternary hyperstructures associated with chain reactions.

1 Introduction

Algebraic hyperstructures represent a natural extension of classical algebraic structures and they were introduced in 1934 by the French mathematician F. Marty [10]. 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. Since then, hundreds of papers and several books have been written on this topic. One of the first books, dedicated especially to hypergroups, is "*Prolegomena of Hypergroup Theory*", written by P. Corsini in 1993 [2]. Another book on "*Hyperstructures and Their Representations*", by T. Vougiouklis, was published one year later [15].

On the other hand, algebraic hyperstructure theory has a multiplicity of applications to other disciplines: geometry, graphs and hypergraphs, binary relations, lattices, groups, fuzzy sets and rough sets, automata, cryptography, codes, median algebras, relation algebras, C-algebras, artificial intelligence, probabilities and so on. A recent book on these topics is "*Applications of Hyperstructure Theory*", by P. Corsini and V. Leoreanu, published by Kluwer Academic Publishers in 2003 [3]. We mention here another important book for the applications in Geometry and for the clearness of the exposition, written by W. Prenowitz and J. Jantosciak [12]. Another monograph is devoted especially to the study of Hyperring Theory, written by Davvaz and Leoreanu-Fotea [4]. It begins with some basic results concerning ring theory and algebraic hyperstructures, which represent the most general algebraic context, in which the reality can be modelled. Several kinds of hyperrings are introduced and analyzed in this book. The volume ends with an outline of applications in Chemistry (also see [5]) and Physics, canalizing several special kinds of hyperstructures: e-hyperstructures and transposition hypergroups. The theory of suitable modified hyperstructures can serve as a mathematical background in the field of quantum communication systems.

n-ary generalizations of algebraic structures is the most natural way for further development and deeper understanding of their fundamental properties. In [6], Davvaz and Vougiouklis introduced the concept of n-ary hypergroups as a generalization of hypergroups in the sense of Marty. Also, we can consider n-ary hypergroups as a nice generalization of n-ary groups. Leoreanu-Fotea and Davvaz in [8] introduced and studied the notion of a partial n-ary hypergroupoid, associated with a binary relation. Some important results, concerning Rosenberg partial hypergroupoids, induced by relations, are generalized to the case of n-ary hypergroupoids, also see [9]. Ternary semihypergroups are algebraic structures with one associative hyperoperation. A ternary semihypergroup is a particular case of an n-ary semihypergroup (n-semihypergroup) for $n = 3$.

The main purpose of this paper is to provide examples of ternary hyperstructures associated with chain reactions.

2 Algebraic hyperstructures

2.1 Binary algebraic hyperstructures

An *algebraic hyperstructure* is a non-empty set H together with a function $\cdot : H \times H \longrightarrow \wp^*(H)$ called *hyperoperation*, where $\wp^*(H)$ denotes the set of all non-empty subsets of H.

If A, B are non-empty subsets of H and $x \in H$, then we define

$$A \cdot B = \bigcup_{a \in A, b \in B} a \cdot b, \quad x \cdot B = \{x\} \cdot B, \quad \text{and} \quad A \cdot x = A \cdot \{x\} .$$

The hyperoperation $(\cdot)$ is called *associative* in H if

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

which means that

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

We say that a semihypergroup $(H, \otimes)$ is a *hypergroup* if for all $x \in H$, we have $x \cdot H = H \cdot x = H$. A hypergroupoid $(H, \cdot)$ is an H_v*-group*, if for all $x, y, z \in H$, the following conditions hold:

(1) $x \cdot (y \cdot z) \cap (x \cdot y) \cdot z \neq \emptyset$,

(2) $x \cdot H = H \cdot x = H$.

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 $a \in K$.

2.2 Ternary algebraic hyperstructures

Let H be a non-empty set and $f : H \times H \times H \longrightarrow \wp^*(H)$, where $\wp^*(H)$ is the set of all non-empty subsets of H. Then f is called a *ternary hyperoperation* on H and the pair (H, f) is called a ternary hypergroupoid. If A, B, C are non-empty subsets of H, then we define

$$f(A, B, C) = \bigcup_{a \in A, b \in B, c \in C} f(a, b, c).$$

A ternary hypergroupoid (H, f) is called a *ternary semihypergroup* if for every $a_1, \dots a_5 \in H$, we have

$$f(f(a_1, a_2, a_3), a_4, a_5) = f(a_1, f(a_2, a_3, a_4), a_5) = f(a_1, a_2, f(a_3, a_4, a_5)) .$$

A non-empty set H together with a ternary hyperoperation f is called a *ternary* H_v*-semigroup* if the *weak associativity* is valid, i.e., for every $a_1, \dots a_5 \in H$,

$$f(f(a_1, a_2, a_3), a_4, a_5) \cap f(a_1, f(a_2, a_3, a_4), a_5) \cap f(a_1, a_2, f(a_3, a_4, a_5)) \neq \emptyset .$$

Since we can identify the set $\{x\}$ with the element x, any ternary semigroup is a ternary semihypergroup. A ternary semigroup does not necessarily reduce to an ordinary semigroup. This has been shown by the following example. Let $S = \{-i, 0, i\}$ be a ternary semigroup under the multiplication over complex numbers whole S is not a binary semigroup under the multiplication over complex numbers [7].

A ternary semihypergroup (respectively, ternary $H - v$-semigroup) (H, f) is called a *ternary hypergroup* (respectively, ternary $H - v$-group) if for all $a, b, c \in H$ there exist $x, y, z \in H$ such that:

$$c \in f(x, a, b) \cap f(a, y, b) \cap f(a, b, z).$$

Notice that a ternary semigroup (S, f) is said to be a *ternary group* if it satisfies the following property that for all $a, b, c \in S$, there exist unique $x, y, z \in S$ such that

$$c = f(x, a, b), \quad c = f(a, y, b), \quad c = f(a, b, z)\ .$$

Therefore, a ternary group is a ternary hypergroup, too.

3 Chain reactions

3.1 Radical

An atom or group of atoms possessing an odd (unpaired) electron is called radical. Radical species can be electrically neutral, in which case they are sometimes referred to as free radicals. Pairs of electrically neutral "free" radicals are formed via homolytic bond breakage. This can be achieved by heating in non-polar solvents or the vapor phase. At elevated temperature or under the influence ultraviolet light at room tempreture, all molecular species will dissociate into radicals. Homolsis or homolytic bond fragmentation occurs when (in the language of Lewis theory) a two electron covalent bond breaks and one electron goes to each of the partner species.

For example, chlorine, Cl_2, forms chlorine radicals $(Cl^{\bullet})$ and peroxides form oxygen radicals.

$$X\text{—}X \longrightarrow 2X^{\bullet}$$
$$Cl\text{—}Cl \longrightarrow 2Cl^{\bullet}$$
$$R\text{—}O\text{—}O\text{–}R \longrightarrow R\text{—}O^{\bullet}$$

3.2 Radical reactions

Radical bond forming reactions (radical couplings) are rather rare processes. The reason is because radicals are normally present at low concentrations in a reaction medium, and it is statistically more likely they will abstract a hydrogen, or undergo another type of a substitution process, rather than reacting with each other by coupling. And as radicals are uncharged, there is little long range Coulombic attraction between two radical centres.

Radical substitution reactions tend to proceed as chain reaction processes, often with many thousands of identical propagation steps. The propensity for chain reactivity gives radical chemistry a distinct feel compared with polar Lewis acid/base chemistry where chain reactions are less common.

3.3 Chain radical substitution

Methane can be chlorinated with chlorine to give chloromethane and hydrogen chloride. The reaction proceeds as a chain, radical, substitution mechanism. The process is a little more involved, and three steps are involved: initiation, propagation and termination:

(1) $Cl_2 \longrightarrow 2Cl^\bullet$

(1) is called Chain-initiating step.

(2) $Cl^\bullet + CH_4 \longrightarrow HCl + CH_3^\bullet$

(3) $CH_3^\bullet + Cl_2 \longrightarrow CH_3Cl + Cl^\bullet$

then (2), (3), (2), (3), etc, until finally:

(2) and (3) are called Chain-propagating steps.

(4) $Cl^\bullet + Cl^\bullet \longrightarrow Cl_2$ or

(5) $CH_3^\bullet + CH_3^\bullet \longrightarrow CH_3CH_3$ or

(6) $CH_3^\bullet + Cl^\bullet \longrightarrow CH_3Cl$.

(4),(5) and (6) are called Chain-terminating steps.

First in the chain of reactions is a chain-initiating step, in which energy is absorbed and a reactive particle generated; in the present reaction it is the cleavage of chlorine into atoms (step 1).

There are one or more chain-propagating steps, each of which consumes a reactive particle and generates another; there they are the reaction of chlorine atoms with methane (step 2), and of methyl radicals with chlorine (step 3).

A chlorine radical abstracts a hydrogen from methane to give hydrogen chloride and a methyl radical. The methyl radical then abstracts a chlorine atom (a chlorine radical) from Cl_2 to give methyl chloride and a chlorine radical... which abstracts a hydrogen from methane... and the cycle continues... Finally there are chain-terminating steps, in which reactive particles are consumed but not generated; in the chlorination of methane these would involve the union of two of the reactive particles, or the capture of one of them by the walls of the reaction vessel.

3.4 The Halogens F, Cl, Br, and I

The halogens are all typical non-metals. Although their physical forms differ-fluorine and chlorine are gases, bromine is a liquid and iodine is a solid at room temperature, each consists of diatomic molecules; F_2, Cl_2, Br_2 and I_2. The halogens all react with hydrogen to form gaseous compounds, with the formulas HF, HCl, HBr, and HI all of which are very soluble in water. The halogens all react with metals to give halides.

$$:\ddot{\underset{..}{F}}\ \text{-}\ \ddot{\underset{..}{F}}:,\qquad :\ddot{\underset{..}{Cl}}\ \text{-}\ \ddot{\underset{..}{Cl}}:,\qquad :\ddot{\underset{..}{Br}}\ \text{-}\ \ddot{\underset{..}{Br}}:,\qquad :\ddot{\underset{..}{I}}\ \text{-}\ \ddot{\underset{..}{I}}:$$

The reader will find in [11] a deep discussion of chain reactions and halogens.

4 Chemical algebraic hyperstructures

In during chain reaction

$$A_2 + B_2 \overset{\text{Heat or Light}}{\longleftrightarrow} 2AB$$

there exist all molecules A_2, B_2, AB and whose fragment parts $A^\bullet, B^\bullet$ in experiment. Elements of this collection can by combine with each other. All combinational probabilities for the set $H = \{A^\bullet, B^\bullet, A_2, B_2, AB\}$ to do without energy can be displayed as follows:

$+$	$A^\bullet$	$B^\bullet$	A_2	B_2	AB
$A^\bullet$	$A^\bullet, A_2$	$A^\bullet, B^\bullet, AB$	$A^\bullet, A_2$	$A^\bullet, B_2, B^\bullet, AB$	$A^\bullet, AB, A_2, B^\bullet$
$B^\bullet$	$A^\bullet, B^\bullet, AB$	$B^\bullet, B_2$	$A^\bullet, B^\bullet, AB, A_2$	$B^\bullet, B_2$	$A^\bullet, B^\bullet, AB, B_2$
A_2	$A^\bullet, A_2$	$A^\bullet, B^\bullet, AB, A_2$	$A^\bullet, A_2$	$A^\bullet, B^\bullet, A_2, B_2, AB$	$A^\bullet, B^\bullet, A_2, AB$
B_2	$A^\bullet, B^\bullet, B_2, AB$	$B^\bullet, B_2$	$A^\bullet, B^\bullet, A_2, B_2, AB$	$B^\bullet, B_2$	$A^\bullet, B^\bullet, B_2, AB$
AB	$A^\bullet, AB, A_2, B^\bullet$	$A^\bullet, B^\bullet, AB, B_2$	$A^\bullet, B^\bullet, A_2, AB$	$A^\bullet, B^\bullet, B_2, AB$	$A^\bullet, B^\bullet, A_2, B_2, AB$

Theorem. $(H,+)$ is an H_v-group.

$X = \{A^\bullet, A_2\}$ and $Y = \{B^\bullet, B_2\}$ are only H_v-subgroups of $(H,+)$.

If we consider $A = H$ and $B \in \{F, CL, Br, I\}$ (for example $B = I$), the complete reaction table becomes:

$+$	$H^\bullet$	$I^\bullet$	H_2	I_2	HI
H^o	$H^\bullet, H_2$	$H^\bullet, I^\bullet, HI$	$H^\bullet H_2$	$H^\bullet, I_2, I^\bullet, HI$	$H^\bullet, HI, H_2, I^\bullet$
$I^\bullet$	$H^\bullet, I^\bullet, HI$	$I^\bullet, I_2$	$H^\bullet, I^\bullet, HI, H_2$	$I^\bullet, I_2$	$H^\bullet, I^\bullet, HI, I_2$
H_2	$H^\bullet, H_2$	$H^\bullet, I^\bullet, HI, I_2$	$H^\bullet, H_2$	$H^\bullet, I^\bullet, H_2, I_2, HI$	$H^\bullet, I^\bullet, H_2, HI$
I_2	$H^\bullet, I^\bullet, I_2, HI$	$H^\bullet, I_2$	$H^\bullet, I^\bullet, H_2, I_2, HI$	$H^\bullet, I_2$	$H^\bullet, I^\bullet, I_2, HI$
HI	$H^\bullet, HI, H_2, I^\bullet$	$H^\bullet, I^\bullet, HI, I_2$	$H^\bullet, I^\bullet, H_2, HI$	$H^\bullet, I^\bullet, H_2, HI$	$H^\bullet, I^\bullet, H_2, I_2, HI$

Now, we consider the ternary combinations:

$f(A^\bullet, -, -)$	$A^\bullet$	$B^\bullet$	A_2	B_2	AB
$A^\bullet$	$A^\bullet, A_2$	$A^\bullet, B^\bullet, A_2, AB$	$A^\bullet, A_2$	H	$A^\bullet, AB, A_2, B^\bullet$
$B^\bullet$	$A^\bullet, B^\bullet, A_2, AB$	$A^\bullet, B^\bullet, B_2, AB$	$A^\bullet, B^\bullet, AB, A_2$	$A^\bullet, B^\bullet, B_2, AB$	H
A_2	$A^\bullet, A_2$	$A^\bullet, B^\bullet, AB, A_2$	$A^\bullet, A_2$	H	$A^\bullet, B^\bullet, A_2, AB$
B_2	$A^\bullet, B^\bullet, B_2, AB$	$A^\bullet, B^\bullet, B_2, AB$	H	$A^\bullet, B^\bullet, B_2, AB$	H
AB	$A^\bullet, B^\bullet, A_2, AB$	H	$A^\bullet, B^\bullet, A_2, AB$	H	H

$f(B^\bullet, -, -)$	$A^\bullet$	$B^\bullet$	A_2	B_2	AB
$A^\bullet$	$A^\bullet, A_2, B^\bullet, AB$	$A^\bullet, B^\bullet, B_2, AB$	$A^\bullet, A_2, B^\bullet, AB$	$A^\bullet, B_2, B^\bullet, AB$	H
$B^\bullet$	$A^\bullet, B^\bullet, B_2, AB$	$B^\bullet, B_2$	H	$B^\bullet, B_2$	$A^\bullet, B^\bullet, AB, B_2$
A_2	$A^\bullet, A_2, B^\bullet, AB$	H	$A^\bullet, A_2, B^\bullet, AB$	H	H
B_2	$A^\bullet, B^\bullet, B_2, AB$	$B^\bullet, B_2$	H	$B^\bullet, B_2$	$A^\bullet, B^\bullet, B_2, AB$
AB	H	$A^\bullet, B^\bullet, AB, B_2$	H	$A^\bullet, B^\bullet, B_2, AB$	H

$f(A_2, -, -)$	$A^\bullet$	$B^\bullet$	A_2	B_2	AB
$A^\bullet$	$A^\bullet, A_2$	$A^\bullet, B^\bullet, A_2, AB$	$A^\bullet, A_2$	H	$A^\bullet, AB, A_2, B^\bullet$
$B^\bullet$	$A^\bullet, B^\bullet, A_2, AB$	H	$A^\bullet, B^\bullet, AB, A_2$	H	H
A_2	$A^\bullet, A_2$	$A^\bullet, B^\bullet, AB, A_2$	$A^\bullet, A_2$	H	$A^\bullet, B^\bullet, A_2, AB$
B_2	H	H	H	H	H
AB	$A^\bullet, A_2, B^\bullet, AB$	H	$A^\bullet, B^\bullet, A_2, AB$	H	H

$f(B_2, -, -)$	$A^\bullet$	$B^\bullet$	A_2	B_2	AB
$A^\bullet$	H	$A^\bullet, B^\bullet, B_2, AB$	H	$A^\bullet, B_2, B^\bullet, AB$	H
$B^\bullet$	$A^\bullet, B^\bullet, B_2, AB$	$B^\bullet, B_2$	H	$B^\bullet, B_2$	$A^\bullet, B^\bullet, AB, B_2$
A_2	H	H	H	H	H
B_2	$A^\bullet, B^\bullet, B_2, AB$	$B^\bullet, B_2$	H	$B^\bullet, B_2$	$A^\bullet, B^\bullet, B_2, AB$
AB	H	$A^\bullet, B^\bullet, AB, B_2$	H	$A^\bullet, B^\bullet, B_2, AB$	H

$f(AB, -, -)$	$A^\bullet$	$B^\bullet$	A_2	B_2	AB
$A^\bullet$	$A^\bullet, A_2, B^\bullet, AB$	H	$A^\bullet, A_2, B^\bullet, AB$	H	H
$B^\bullet$	H	$A^\bullet, B_2, B^\bullet, AB$	H	$A^\bullet, B_2, B^\bullet, AB$	H
A_2	$A^\bullet, A_2, B^\bullet, AB$	H	$A^\bullet, A_2, B^\bullet, AB$	H	H
B_2	H	$A^\bullet, B_2, B^\bullet, AB$	H	$A^\bullet, B_2, B^\bullet, AB$	H
AB	H	H	H	H	H

Theorem. (H, f) is a ternary H_v-group.

As a simple of how to calculate the associativity, we illustrate one of the cases:

$$\begin{aligned}
&f(f(A^\bullet, A_2, AB), A^\bullet, A^\bullet) = f(\{A^\bullet, B^\bullet, A_2, AB\}, A^\bullet, A^\bullet)\\
&= f(A^\bullet, A^\bullet, A^\bullet) \cup f(B^\bullet, A^\bullet, A^\bullet) \cup f(A_2, A^\bullet, A^\bullet) \cup f(AB, A^\bullet, A^\bullet)\\
&= \{A^\bullet, A_2\} \cup \{A^\bullet, A_2, B^\bullet, AB\} \cup \{A^\bullet, A_2\} \cup \{A^\bullet, A_2, B^\bullet, AB\}\\
&= \{A^\bullet, A_2, B^\bullet, AB\},
\end{aligned}$$

$$\begin{aligned}
&f(A^\bullet, f(A_2, AB, A^\bullet), A^\bullet) = f(A^\bullet, \{A^\bullet, A_2, B^\bullet, AB\}, A^\bullet)\\
&= f(A^\bullet, A^\bullet, A^\bullet) \cup f(A^\bullet, A_2, A^\bullet) \cup f(A^\bullet, B^\bullet, A^\bullet) \cup f(A^\bullet, AB, A^\bullet)\\
&= \{A^\bullet, A_2\} \cup \{A^\bullet, A_2\} \cup \{A^\bullet, A_2, B^\bullet, AB\} \cup \{A^\bullet, A_2, B^\bullet, AB\}\\
&= \{A^\bullet, A_2, B^\bullet, AB\}
\end{aligned}$$

and

$$\begin{aligned}
&f(A^\bullet, A_2, f(AB, A^\bullet, A^\bullet)) = f(A^\bullet, A_2, \{A^\bullet, A_2, B^\bullet, AB\})\\
&= f(A^\bullet, A_2, A^\bullet) \cup f(A^\bullet, A_2, A_2) \cup f(A^\bullet, A_2, B^\bullet) \cup f(A^\bullet, A_2, AB)\\
&= \{A^\bullet, A_2\} \cup \{A^\bullet, A_2\} \cup \{A^\bullet, A_2, B^\bullet, AB\} \cup \{A^\bullet, A_2, B^\bullet, AB\}\\
&= \{A^\bullet, A_2, B^\bullet, AB\}.
\end{aligned}$$

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