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Hypergroups Obtained from Formation Reaction of Simple Gas Hydrates

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Abstract

Gas hydrates have potential for many industrial applications. In this paper, we study the formation reaction of simple gas hydrates by modeling them using algebraic hyperstructures theory. In this way, we show that the factors forming this reaction can be seen as a commutative (ternary) hypergroup which is not a join (ternary) space.

1 Introduction

One useful extensions in algebra is algebraic hyperstructures theory, which was introduced by Marty in [25]. This can be confirmed by hyperstructure applications to several domains of mathematics and other sciences such as geometry, groups, graphs, median algebras, relation algebras, C-algebras, Boolean algebras, categories, topology, binary relations, lattices, fuzzy sets, rough and soft sets, automata, coding theory, cryptography, probability, artificial intelligence, dynamical systems, physic, chemistry and etc. For an overview of the theory and its applications, we can see [6–9, 16, 33].

Applications in chemistry refers to chemical reactions. 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. It can be a useful tool for mathematical modeling of a set of chemical elements under a chemical reaction. Since the number of elements released under a chemical reaction may be more than one, it seems that classical algebraic structures are not appropriate in this case. For example, obtained results in this paper can be exposed through hypergroups, not groups. Studies on representation of obtained combinations from chemical reactions as algebraic hyperstructures have been done till now for chain reactions in [10], dismutation reactions in [11], redox reactions in [14], radiolytic processes in cement medium in [15], standard reduction potentials for three consecutive oxidation states of elements in [5], chemical reactions for iron and indium in [3] and also for vanadium in [4]. Moreover, using n-ary hypergroups ([18]), which are a generalization of hypergroups, chain, dismutation and redox reactions were studied in [12, 13, 17], respectively.

In this paper, formation reaction of simple gas hydrates are studied and we show that they can be modeled as commutative hypergroups, which are not join spaces. Also, we investigate them in form of ternary hypergroups (3-ary hypergroups).

2 Basic concepts of hypergroups and join spaces

A non-empty set H together with the function $\circ : H \times H \longrightarrow \mathcal{P}^*(H)$ is called a *hyperoperation*, where $\mathcal{P}^*(H)$ is the set of all non-empty subsets of H. In this case, $(H, \circ)$ is said to be a *hypergroupoid*, the simplest algebraic hyperstructure. For the non-empty subsets A and B of H we define $A \circ B = \bigcup\limits_{a\in A,\ b\in B} a \circ b$. Also, if $x \in H$, we have $A \circ x = A \circ \{x\}$ and $x \circ B = \{x\} \circ B$.

A pair $(H, \circ)$ is called a *hypergroup* if it is satisfied in the following conditions:

(1) $(H, \circ)$ is a *semihypergroup*. Indeed, the hyperoperation " $\circ$ " is associative on H, that is $(x \circ y) \circ z = x \circ (y \circ z)$ for all $x, y, z \in H$, which means that

$$\bigcup_{a\in x\circ y} a \circ z = \bigcup_{b\in y\circ z} x \circ b;$$

(2) for all $x \in H$ we have $x \circ H = H = H \circ x$ (reproduction axiom).

A non-empty subset K of H is said to be a *subhypergroup* if $a \circ K = K = K \circ a$ for all $a \in K$.

Let $a, b \in H$ and consider a hyperoperation "$\circ$" on H. Define $a/b = \{t \in H \mid a \in t \circ b\}$. A commutative hypergroup $(H, \circ)$ is called a *join space* if for all $a, b, c, d \in H$ we have

$$a/b \ \cap \ c/d \neq \emptyset \implies a \circ d \ \cap \ b \circ c \neq \emptyset.$$

For two hypergroups $(H, \circ)$ and $(T, *)$, a function $f : H \longrightarrow T$ is said to be

(i) a *homomorphism*, if $f(a \circ b) \subseteq f(a) * f(b)$, for all $a, b \in H$.

(ii) a *strong homomorphism*, if for all $a, b \in H$ we have $f(a \circ b) = f(a) * f(b)$.

Moreover, we write $H \cong T$ if there exists a strong homomorphism $f : H \longrightarrow T$ such that f is one to one and onto.

Now, for a non-empty set H, define the map $f : H \times H \times H \longrightarrow \mathcal{P}^*(H)$. Then f is called a *ternary hyperoperation* and (H, f) a *ternary hypergroupoid.* In this case, we have

$$f(A, B, C) = \bigcup_{x \in A, y \in B, z \in C} f(x, y, z),$$

for all $A, B, C \subseteq H$. The ternary hyperperation f is said to be commutative, if $f(x_1, x_2, x_3) = f(x_{\sigma(1)}, x_{\sigma(2)}, x_{\sigma(3)})$ for all $\sigma \in \mathbb{S}_3$ and $x_1, x_2, x_3 \in H$.

We say that a ternary hypergroupoid (H, f) is a *ternary hypergroup*, if

(1) for all $x_1, x_2, \ldots, x_5 \in H$ we have

$$f(f(x_1, x_2, x_3), x_4, x_5) = f(x_1, f(x_2, x_3, x_4), x_5) = f(x_1, x_2, f(x_3, x_4, x_5)).$$

(2) $f(H, y, z) = f(x, H, z) = f(x, y, H) = H$ for all $x, y, z \in H$.

A non-empty K is a subhypergroup of ternary hypergroup (H, f) if $f(K, y, z) = f(x, K, z) = f(x, y, K) = K$ for all $x, y, z \in K$.

Moreover, a commutative ternary hypergroup (H, f) is a *join ternary space*, if $(a/b, c) \cap (x/y, z) \neq \emptyset$ implies that $f(a, y, z) \cap f(x, b, c) \neq \emptyset$, for all $a, b, c, x, y, z \in H$, where $(a/b, c) = \{t \in H \mid a \in f(t, b, c)\}$.

3 Formation reaction of simple gas hydrates

Gas hydrates, also known as clathrate hydrates, are nonstoichiometric crystalline compounds formed when gas (guest) molecules of certain size comes into contact with water (host) at relatively low temperatures and high pressures [31]. Examples of guest molecules are methane, ethane, carbon dioxide, hydrogen sulfide, propane, natural gas, and some small organic molecules such as acetone, tetrahydrofuran, and cyclopentane [26]. Guest molecules are encapsulated in a host lattice of hydrogen-bonded water molecules to form clathrate gas hydrates [29, 31].

There are three common structures for gas hydrate molecules: cubic structure I (SI), cubic structure II (SII), and hexagonal structure H (SH) [30, 31]. For each of the three types, different gases are stable within the cage due to the varying shape and size of the vacancies. Structure SI consists of two pentagonal dodecahedron (5^{12}) cages and six tetrakaidekahedron ($5^{12}6^2$) cages with a total of 46 water molecules per unit cell [20, 31]. Structure SII comprises sixteen pentagonal dodecahedron (5^{12}) cages and eight hexakaidecahedron ($5^{12}6^4$) cages, with 136 water molecules. Structure SH has three pentagonal dodecahedron (5^{12}) cages, two irregular dodecahedron ($4^35^66^3$) cages and one icosahedron ($5^{12}6^8$) cage, with a total of 34 water molecules [20, 31]. Table 1 lists the hydration numbers of various hydrate structures and some of SI, SII, and SH hydrate formers, where "n" is the number of water molecules per guest molecule, and "M" shows a hydrate former (guest).

Table 1. The hydration numbers of various hydrate structures and some of SI, SII, and SH hydrate formers.

structure	SI	SII	SH
Hydration number (n)	5.75	5.67	5.67
M	Xe, Cl_2 CO_2, N_2O H_2Se, SO_2 CH_4, C_2H_4 CH_3F, CH_2F_2 CH_4, C_2H_3F CH_3CHF_2 BrCl, H_2S C_2H_6, COS C_2H_5F, CHF_3	Ar, Kr, H_2 N_2, O_2, C_3H_8 $(CH_3)_3CF$ Propylene Cyclopentene iso-butane	2-Methylbutane, 2, 2-Dimethylbutan 2, 3-Dimethylbutane 2, 2, 3-Trimethylbutane 2, 2-Dimethylpentane 3, 3-Dimethylpentane Ethylcyclopentane Methylcyclohexane Methylcyclopentane 1, 1-Dimethylcyclohexane Cycloheptane 2, 3-Dimethyl-1-butene

When Priestly first discovered hydrates in 1778, they were studied mainly out of scientific curiosity. In 1934, Hammerschmidt determined that hydrates were plugging natural gas transmission lines. This marked the beginning of hydrate research in the oil and gas industry [21]. Due to high gas and energy storage capacity of gas hydrates and its potential for separation processes, great attention has been paid to the positive application of this technology (such as natural gas storage and transportation, gas separation, energy storage, water desalination, refrigeration systems, and so on [1,2,19,22–24,27,28,32]), in recent years.

In the process of gas hydrate formation, the reaction of a gas with water can be expressed as follows [31]:

$$M + nH_2O \leftrightharpoons M(H_2O)_n,$$

where M stands for a gas (hydrate former) and n is the hydration number. Gas hydrates can form in high-pressure, low-temperature conditions where free water is present. Figure 1 shows the hydrate formation conditions of some hydrate formers. As can be seen in this figure, the hydrate formation conditions of various gases are different. Some gases such as nitrogen and methane can form gas hydrate at very high pressures and low temperatures and some of them such as hydrogen sulfide and propane form hydrate at relatively moderate conditions.

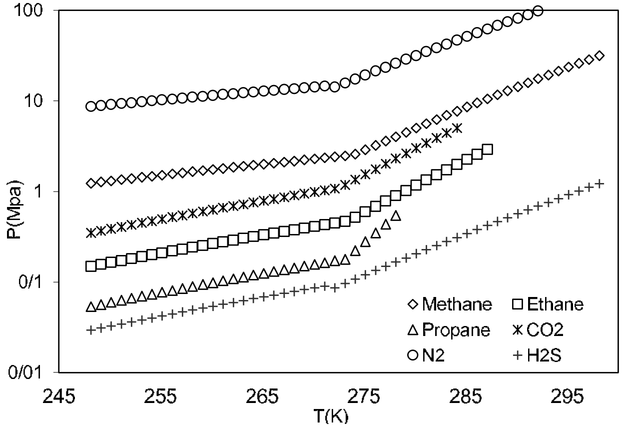

Figure 1. the hydrate formation conditions of some hydrate formers

As shown in the hydrate formation reaction, there are three components in this process: water (H_2O), gas (M), and gas hydrate ($M(H_2O)_n$). All possible combinations for the set $\mathcal{T} = \{M, H_2O, M(H_2O)_n\}$ under the hydrate formation reaction can be displayed as follows:

$+$	M	H_2O	$M(H_2O)_n$
M	M	$M, H_2O, M(H_2O)_n$	$M, H_2O, M(H_2O)_n$
H_2O	$M, H_2O, M(H_2O)_n$	H_2O	$M, H_2O, M(H_2O)_n$
$M(H_2O)_n$	$M, H_2O, M(H_2O)_n$	$M, H_2O, M(H_2O)_n$	$M, H_2O, M(H_2O)_n$

By renaming of M, H_2O and $M(H_2O)_n$ as

$$M := a, \quad H_2O := b, \quad M(H_2O)_n := c,$$

we obtain the following table:

$+$	a	b	c
a	a	$\mathcal{T}$	$\mathcal{T}$
b	$\mathcal{T}$	b	$\mathcal{T}$
c	$\mathcal{T}$	$\mathcal{T}$	$\mathcal{T}$

Then, it can be seen that $(\mathcal{T}, +)$ is a commutative hypergroup. Indeed, clearly, $+$ is commutative. Also, we have

$(a+a)+a = a+a = a$	$a+(a+a) = a+a = a$
$(a+a)+b = a+b = \mathcal{T}$	$a+(a+b) = a+\mathcal{T} = \mathcal{T}$
$(a+a)+c = a+c = \mathcal{T}$	$a+(a+c) = a+\mathcal{T} = \mathcal{T}$
$(b+b)+a = b+a = \mathcal{T}$	$b+(b+a) = b+\mathcal{T} = \mathcal{T}$
$(b+b)+b = b+b = b$	$b+(b+b) = b+b = b$
$(b+b)+c = b+c = \mathcal{T}$	$b+(b+c) = b+\mathcal{T} = \mathcal{T}$
$(c+c)+a = \mathcal{T}+a = \mathcal{T}$	$c+(c+a) = c+\mathcal{T} = \mathcal{T}$
$(c+c)+b = c+b = \mathcal{T}$	$c+(c+b) = c+\mathcal{T} = \mathcal{T}$
$(c+c)+c = c+c = \mathcal{T}$	$c+(c+c) = c+c = \mathcal{T}$
$(a+b)+c = \mathcal{T}+c = \mathcal{T}$	$a+(b+c) = a+\mathcal{T} = \mathcal{T}$
$(a+c)+b = \mathcal{T}+b = \mathcal{T}$	$a+(c+b) = a+\mathcal{T} = \mathcal{T}$

Hence, we can see that $+$ is associative on $\mathcal{T}$. Moreover, $x + \mathcal{T} = \mathcal{T}$, for all $x \in \mathcal{T}$. So,

Theorem 3.1. $(\mathcal{T}, +)$ *is a commutative hypergroup.*

Furthermore, notice that for $M := a$ and $H_2O := b$ of $\mathcal{T}$, we have

$$a/b = \{t \mid a \in t + b\} = \{a, c\} \ \text{ and } \ b/a = \{z \mid b \in z + a\} = \{b, c\},$$

which imply that $a/b \ \cap \ b/a \neq \emptyset$. But $a + a \ \cap \ b + b = \{a\} \cap \{b\} = \emptyset$. Hence, the commutative hypergroup $(\mathcal{T}, +)$ is not a join space.

In addition, the sets $\{a\}$ and $\{b\}$ are only subhypergroups of $(\mathcal{T}, +)$, which we have $(\{a\}, +) \cong (\{b\}, +)$.

Therefore, every element of Table 1 with related hydration number under the hydrate formation reaction can construct a commutative hypergroup. Hence, many properties of hypergroups, according to [6–9, 16, 33], can be expressed for simple gas hydrates.

Now, for example consider $M := Ar$ with hydration number $n = 5.67$, then we have the following table for hydrate formation reaction of it:

$+$	Ar	H_2O	$Ar(H_2O)_{5.67}$
Ar	Ar	$Ar, H_2O, Ar(H_2O)_{5.67}$	$Ar, H_2O, Ar(H_2O)_{5.67}$
H_2O	$Ar, H_2O, Ar(H_2O)_{5.67}$	H_2O	$Ar, H_2O, Ar(H_2O)_{5.67}$
$Ar(H_2O)_{5.67}$	$Ar, H_2O, Ar(H_2O)_{5.67}$	$Ar, H_2O, Ar(H_2O)_{5.67}$	$Ar, H_2O, Ar(H_2O)_{5.67}$

Hence, for ternary combinatorics we have:

$f(Ar, -, -)$	Ar	H_2O	$Ar(H_2O)_{5.67}$
Ar	Ar	$Ar, H_2O, Ar(H_2O)_{5.67}$	$Ar, H_2O, Ar(H_2O)_{5.67}$
H_2O	$Ar, H_2O, Ar(H_2O)_{5.67}$	$Ar, H_2O, Ar(H_2O)_{5.67}$	$Ar, H_2O, Ar(H_2O)_{5.67}$
$Ar(H_2O)_{5.67}$	$Ar, H_2O, Ar(H_2O)_{5.67}$	$Ar, H_2O, Ar(H_2O)_{5.67}$	$Ar, H_2O, Ar(H_2O)_{5.67}$

$f(H_2O, -, -)$	Ar	H_2O	$Ar(H_2O)_{5.67}$
Ar	$Ar, H_2O, Ar(H_2O)_{5.67}$	$Ar, H_2O, Ar(H_2O)_{5.67}$	$Ar, H_2O, Ar(H_2O)_{5.67}$
H_2O	$Ar, H_2O, Ar(H_2O)_{5.67}$	H_2O	$Ar, H_2O, Ar(H_2O)_{5.67}$
$Ar(H_2O)_{5.67}$	$Ar, H_2O, Ar(H_2O)_{5.67}$	$Ar, H_2O, Ar(H_2O)_{5.67}$	$Ar, H_2O, Ar(H_2O)_{5.67}$

$f(Ar(H_2O)_{5.67}, -, -)$	Ar	H_2O	$Ar(H_2O)_{5.67}$
Ar	$Ar, H_2O, Ar(H_2O)_{5.67}$	$Ar, H_2O, Ar(H_2O)_{5.67}$	$Ar, H_2O, Ar(H_2O)_{5.67}$
H_2O	$Ar, H_2O, Ar(H_2O)_{5.67}$	$Ar, H_2O, Ar(H_2O)_{5.67}$	$Ar, H_2O, Ar(H_2O)_{5.67}$
$Ar(H_2O)_{5.67}$	$Ar, H_2O, Ar(H_2O)_{5.67}$	$Ar, H_2O, Ar(H_2O)_{5.67}$	$Ar, H_2O, Ar(H_2O)_{5.67}$

By $\mathcal{T} = \{Ar, H_2O, Ar(H_2O)_{5.67}\}$, it can be seen that $(\mathcal{T}, f)$ is a commutative ternary hypergroup.

We illustrate one of the cases about associativity of f:

$$f\Big(f(Ar, Ar, Ar), H_2O, Ar(H_2O)_{5.67}\Big) = f(Ar, H_2O, Ar(H_2O)_{5.67}) = \mathcal{T}$$

$$f\Big(Ar, f(Ar, Ar, H_2O), Ar(H_2O)_{5.67}\Big) = f(Ar, \mathcal{T}, Ar(H_2O)_{5.67}\Big) = \mathcal{T}$$

$$f\Big(Ar, Ar, f(Ar, H_2O, Ar(H_2O)_{5.67})\Big) = f(Ar, Ar, \mathcal{T}\Big) = \mathcal{T}$$

Similarly, we can see the associativity of f in all cases.

Also, we have $f(Ar, Ar, Ar) = \{Ar\}$ and $f(H_2O, H_2O, H_2O) = \{H_2O\}$. Moreover, $(Ar/H_2O, H_2O) = \{t \in \mathcal{T} \mid Ar \in f(t, H_2O, H_2O)\} = \{Ar, Ar(H_2O)_{5.67}\}$ and

$(H_2O/Ar, Ar) = \{z \in \mathcal{T} \mid H_2O \in f(z, Ar, Ar)\} = \{H_2O, Ar(H_2O)_{5.67}\}$. Therefore, $(Ar/H_2O, H_2O) \cap (H_2O/Ar, Ar) \neq \emptyset$ while $f(Ar, Ar, Ar) \cap f(H_2O, H_2O, H_2O) = \emptyset$, and so $(\mathcal{T} = \{Ar, H_2O, Ar(H_2O)_{5.67}\}, f)$ is not a join ternary space.

By a similar manner, it can be shown that for every M with related n based on Table 1, the set $\mathcal{T} = \{M, H_2O, M(H_2O)_n\}$ endowed with ternary hyperoperation f can be seen as commutative ternary hypergroup which is not a join ternary space.

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