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Chemical hyperstructures, superHyperstructures, and SHv-structures: Toward a generalized framework for Hierarchical chemical modeling

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Abstract: The concept of a classical structure provides a broad mathematical framework, whereas a Hyperstructure arises via the powerset construction, and an n-Superhyperstructure is obtained by iterating this construction n times. Intuitively, the n-th powerset corresponds to n successive applications of the powerset operator. Below, we recall the fundamental definitions and illustrate them with elementary examples. In the chemical sciences, various hyperstructural frameworks—such as Chemical Hyperstructures—have also been studied. In this paper, we introduce the notion of a Chemical Superhyperstructure and examine its foundational properties. We further extend the idea of a Weak Chemical Hyperstructure by defining the Weak Chemical Superhyperstructure via the Weak Superhyperstructure (SHv-Structure) framework, and provide an overview of its behavior. These constructions offer a concise and flexible means to represent hierarchical relationships in chemical systems.

Keywords: hyperstructure, superhyperstructure, chemical hyperstructure, chemical superhyperstructure

1. Introduction

1.1. Hyperstructures and superhyperstructures

In this work, the term structure is used in a broad sense: it may refer to any mathematical construct (e.g., graphs, topological spaces, algebraic systems, automata, games) as well as to suitably formalized real-world systems. Many such systems exhibit an intrinsic hierarchical or multi-level organization. In this setting, hyperstructures and superhyperstructures provide particularly expressive modeling tools.

A hyperstructure generalizes a classical algebraic structure by allowing an operation to return a set of possible outputs rather than a single element [1–3]. By iterating the powerset construction, one obtains higher-order domains in which elements themselves are sets (and sets of sets, and so on). This motivates the notion of an n-superhyperstructure [1], which captures multi-layered interactions and provides a natural formalism for hierarchical systems. SuperHyperStructures have attracted considerable research attention in recent years [4–8].

Table 1 summarizes the relationship among classical structures, hyperstructures, superhyperstructures, and (m,n)-superhyperstructures.

Table 1. Classical structures, hyperstructures, (weak) superhyperstructures, and (m,n)-superhyperstructures

Structure type	Carrier (domain)	Typical operation signature
Classical structure	H	$\#_0 : H^m \to H$
Hyperstructure (binary)	H	$\circ : H \times H \to \mathcal{P}^*(H)$
Weak n-superhyperstructure (SHv-structure)	$\mathcal{P}_n(H)$ (or $\mathcal{P}_n^*(H)$)	$\circ : \mathcal{P}_n(H) \times \mathcal{P}_n(H) \to \mathcal{P}^*(\mathcal{P}_n(H))$
(m,n)-superhyperstructure (arity k)	$\mathcal{P}_m(H)$	$\star : (\mathcal{P}_m(H))^k \to \mathcal{P}^*(\mathcal{P}_n(H))$

Notation. $\mathcal{P}(X)$ denotes the powerset of X, and $\mathcal{P}^*(X) = \mathcal{P}(X) \setminus \{\emptyset\}$. We set $\mathcal{P}_0(H) = H$ and $\mathcal{P}_{n+1}(H) = \mathcal{P}(\mathcal{P}_n(H))$. The nonempty iterated powerset removes $\emptyset$ at each stage: $\mathcal{P}_1^*(H) = \mathcal{P}^*(H)$ and $\mathcal{P}_{n+1}^*(H) = \mathcal{P}^*(\mathcal{P}_n^*(H))$. The symbol H^m denotes the m-fold Cartesian product, and k denotes the arity of $\star$.

1.2. Our contributions

In the chemical sciences, several hyperstructural frameworks including chemical hyperstructures have been investigated as a way to encode multi-entity interactions and reaction/affinity relations in a unified language. In this paper, we introduce the notion of a chemical superhyperstructure and study its foundational properties within a powerset-iterated hierarchy.

Moreover, motivated by the notion of a weak chemical hyperstructure, we define a weak chemical superhyperstructure by adopting the weak superhyperstructure (SHv-structure) viewpoint, and we provide an initial account of its behavior and basic examples. These constructions offer a concise and flexible mechanism for representing hierarchical relations in chemical systems, especially when interactions occur simultaneously at multiple organizational levels. For reference, we summarize Chemical HyperStructure vs. Chemical SuperHyperStructure in Table 2, and Chemical SuperHyperStructure vs. Weak Chemical SuperHyperStructure in Table 3.

Table 2. Concise comparison: Chemical HyperStructure vs. Chemical SuperHyperStructure

Aspect	**Chemical HyperStructure**	**Chemical SuperHyperStructure (order n)**
Base domain	G (species)	$\mathcal{P}_n(G)$ (iterated powerset; n-level modules)
Operation type	Hyperoperation $\oplus : G \times G \to \mathcal{P}^*(G)$	Superhyperoperation $\oplus^{(n)} : \mathcal{P}_n(G) \times \mathcal{P}_n(G) \to \mathcal{P}^*(\mathcal{P}_n(G))$
Inputs (reactants)	Two species $x, y \in G$	Two n-level collections $A, B \in \mathcal{P}_n(G)$
Outputs (products)	A nonempty set of species (major products)	A nonempty set of n-level product candidates (pairs $\{y, z\} \subseteq \mathcal{P}_{n-1}(G)$ packaged as elements of $\mathcal{P}_n(G)$)
Selection principle	Choose products maximizing positive ΔE among reactions $x + y \to u + v$	Choose product-modules maximizing positive ΔE among all $a \in A$, $b \in B$ and $a + b \to y + z$
Interpretation	Direct redox products at species level	Hierarchical/coarse-grained redox at module/complex level (symbolic for $n \geq 2$ unless extra constraints are added)
Relationship	—	Reduces to Chemical HyperStructure at $n = 1$ (via singleton embedding)

Table 3. Concise comparison: Chemical SuperHyperStructure vs. Weak Chemical SuperHyperStructure

Aspect	**Chemical SuperHyperStructure (order n)**	**Weak n-Chemical SuperHyperStructure**
Domain	$\mathcal{P}_n(G)$	$\mathcal{P}_n(G)$
Operation / codomain	$\oplus^{(n)} : \mathcal{P}_n(G) \times \mathcal{P}_n(G) \to \mathcal{P}^*(\mathcal{P}_n(G))$	Same operation type/codomain
Defining rule	Maximal positive ΔE selection (major products)	Same maximal-ΔE selection plus a weak associativity axiom
Associativity requirement	Not assumed in general (may be imposed as an extra condition)	Required: $X \oplus^{(n)} (Y \oplus^{(n)} Z) \cap (X \oplus^{(n)} Y) \oplus^{(n)} Z \neq \emptyset$
Algebraic status	An n-superhyperstructure in the sense of having a well-typed operation	An SHv-structure (weak n-superhyperstructure)
Modeling stance	Deterministic rule: "pick strongest" (may still yield multiple maximizers)	Pathway-tolerant: guarantees overlap between different parenthesizations (captures non-unique hierarchical compositions)
Typical use	Hierarchical redox selection without enforcing consistency across bracketing	Hierarchical redox selection with bracketing-robustness / Hv-style behavior

2. Preliminaries

This section introduces the fundamental concepts and definitions that underpin the discussions in this paper. Throughout, all sets are assumed to be finite.

2.1. Classical structure, hyperstructure, and n-superhyperstructure

A Classical Structure represents a general mathematical concept, while a Hyperstructure can be defined using the power set [9–11], and an n-Superhyperstructure can be defined using the n-th powerset [1]. Intuitively, the n-th powerset is a repeated application of the powerset operation. Relevant definitions and simple examples are provided below.

Definition 1 (nth Powerset)**.** (cf. [1,12,13]) Let H be any set. We define its iterated powersets by

$$\mathcal{P}_1(H) = \mathcal{P}(H), \qquad \mathcal{P}_{n+1}(H) = \mathcal{P}\big(\mathcal{P}_n(H)\big) \quad (n \geq 1).$$

Equivalently, one may set $\mathcal{P}_0(H) = H$ and for all $k \geq 0$,

$$\mathcal{P}_{k+1}(H) = \mathcal{P}\big(\mathcal{P}_k(H)\big).$$

The nonempty nth powerset is obtained by removing the empty set at each stage. Writing $\mathcal{P}^*(X) = \mathcal{P}(X) \setminus \{\emptyset\}$, we set

$$\mathcal{P}_1^*(H) = \mathcal{P}^*(H), \qquad \mathcal{P}_{(n+1)}^*(H) = \mathcal{P}^*\big(\mathcal{P}_n^*(H)\big) \quad (n \geq 1).$$

Definition 2 (Classical Structure)**.** (cf. [1,13]) A Classical Structure is a mathematical framework defined on a non-empty set H, equipped with one or more Classical Operations that satisfy specified Classical Axioms. Specifically: A Classical Operation is a function of the form

$$\#_0 : H^m \to H,$$

where $m \geq 1$ is a positive integer, and H^m denotes the m-fold Cartesian product of H. Common examples include addition and multiplication in algebraic structures such as groups, rings, and fields.

Definition 3 (Hyperoperation)**.** (cf. [14,15]) A hyperoperation is a generalization of a binary operation where the result of combining two elements is a set, not a single element. Formally, for a set S, a hyperoperation $\circ$ is defined as

$$\circ : S \times S \to \mathcal{P}(S),$$

where $\mathcal{P}(S)$ is the powerset of S.

Definition 4 (Hyperstructure)**.** (cf. [1,16]) A Hyperstructure extends the notion of a Classical Structure by operating on the powerset of a base set. Formally, it is defined as

$$H = (\mathcal{P}(S), \circ),$$

where S is the base set, $\mathcal{P}(S)$ is the powerset of S, and $\circ$ is an operation defined on subsets of $\mathcal{P}(S)$. Hyperstructures allow for generalized operations that can apply to collections of elements rather than single elements.

Definition 5 (SuperHyperOperations)**.** (cf. [1]) Let H be a non-empty set, and let $\mathcal{P}(H)$ denote the powerset of H. The n-th powerset $\mathcal{P}_n(H)$ is defined recursively as follows:

$$\mathcal{P}_0(H) = H, \qquad \mathcal{P}_{k+1}(H) = \mathcal{P}(\mathcal{P}_k(H)), \quad k \geq 0.$$

A SuperHyperOperation of order (m, n) is an m-ary operation

$$\circ^{(m,n)} : H^m \to \mathcal{P}_n^*(H),$$

where $\mathcal{P}_n^*(H)$ represents the n-th powerset of H, either excluding or including the empty set, depending on the type of operation:

- If the codomain is $\mathcal{P}_n^*(H)$ excluding the empty set, it is called a classical-type (m, n)-SuperHyperOperation.
- If the codomain is $\mathcal{P}_n(H)$ including the empty set, it is called a Neutrosophic (m, n)-SuperHyperOperation.

These SuperHyperOperations are higher-order generalizations of hyperoperations, capturing multi-level complexity through the construction of n-th powersets.

Definition 6 (n-Superhyperstructure)**.** (cf. [1,17]) An n-Superhyperstructure further generalizes a Hyperstructure by incorporating the n-th powerset of a base set. It is formally described as

$$SH_n = (\mathcal{P}_n(S), \circ),$$

where S is the base set, $\mathcal{P}_n(S)$ is the n-th powerset of S, and $\circ$ represents an operation defined on elements of $\mathcal{P}_n(S)$. This iterative framework allows for increasingly hierarchical and complex representations of relationships within the base set.

Example 1 (Drug Formulations as a 2–Superhyperstructure)**.** Let

$$S = \{\text{Aspirin}, \text{Paracetamol}, \text{Caffeine}\}$$

be a set of active pharmaceutical ingredients. We form first–level compounds:

$$C_1 = \{\text{Aspirin}, \text{Caffeine}\}, \qquad C_2 = \{\text{Paracetamol}\} \in \mathcal{P}_1(S).$$

Next, we consider second–level formulations (sets of compounds):

$$F = \{C_1, C_2\} \in \mathcal{P}_2(S).$$

Define a formulation-combination operation

$$\oplus : \mathcal{P}_2(S) \times \mathcal{P}_2(S) \to \mathcal{P}_2(S), \qquad F_1 \oplus F_2 = F_1 \cup F_2.$$

Then $(\mathcal{P}_2(S), \oplus)$ is a 2–Superhyperstructure in which each "formulation" is a set of compounds and the operation $\oplus$ produces new combination therapies by uniting formulations.

2.2. Weak hyperstructure (Hv–structure)

A weak hyperstructure (Hv–structure) is an algebraic system whose hyperoperation satisfies weak associativity: any two ways of bracketing yield intersecting product sets [18,19].

Definition 7 (Weak Hyperstructure (Hv–structure))**.** [20] Let H be a nonempty set and let

$$\cdot : H \times H \to \mathcal{P}^*(H),$$

be a hyperoperation, where $\mathcal{P}^*(H) = \mathcal{P}(H) \setminus \{\emptyset\}$ is the set of all nonempty subsets of H. We say:

1. $\cdot$ is weakly associative if
$$x \cdot (y \cdot z) \cap (x \cdot y) \cdot z \neq \emptyset \qquad \forall x, y, z \in H.$$
2. $\cdot$ is weakly commutative if
$$x \cdot y \cap y \cdot x \neq \emptyset \qquad \forall x, y \in H.$$
3. $(H, \cdot)$ is called an Hv–semigroup if $\cdot$ is weakly associative.
4. $(H, \cdot)$ is called an Hv–group if it is an Hv–semigroup and also satisfies the reproduction axiom:
$$a \cdot H = H \quad \text{and} \quad H \cdot a = H \qquad \forall a \in H.$$

Example 2 (Genetic Inheritance as a Weak Hyperstructure)**.** Let

$$H = \{\text{AA}, \text{Aa}, \text{aa}\},$$

be the set of possible genotypes at a single autosomal locus under Mendelian inheritance. Define a hyperoperation

$$\otimes : H \times H \to \mathcal{P}^*(H),$$

by letting $g_1 \otimes g_2$ be the set of all genotypes that can arise in the offspring when parents of genotypes g_1 and g_2 mate randomly. Concretely, one obtains the following "Punnett-square" hyperoperation table:

$\otimes$	AA	Aa	aa
AA	{AA}	{AA, Aa}	{Aa}
Aa	{AA, Aa}	{AA, Aa, aa}	{Aa, aa}
aa	{Aa}	{Aa, aa}	{aa}

It is straightforward to verify that $(H, \otimes)$ satisfies:

- Weak associativity: for any $x, y, z \in H$, $x \otimes (y \otimes z) \cap (x \otimes y) \otimes z \neq \emptyset$;
- Commutativity: $g_1 \otimes g_2 = g_2 \otimes g_1$ for all g_1, g_2;
- Reproduction axiom (for an Hv–group): $g \otimes H = H = H \otimes g$ for each $g \in H$.

Hence $(H, \otimes)$ is a commutative Hv–group, providing a natural weak hyperstructure model of Mendelian crosses.

2.3. Chemical hyperstructure

A chemical hyperstructure is a hyperalgebraic abstraction of redox interactions, in which each pair of reactants is assigned the (possibly non-unique) set of major products selected by maximizing a positive EMF score.

Definition 8 (Chemical hyperstructure)**.** Let $G = \{X_1, \ldots, X_k\}$ be a finite, nonempty set of chemical species (e.g. oxidation states), and write $\mathcal{P}^*(G) = \mathcal{P}(G) \setminus \{\emptyset\}$. For each ordered pair $(x, y) \in G \times G$, assume we are given a finite set $R(x, y)$ of admissible redox channels. Each channel $r \in R(x, y)$ is of the form

$$r: \; x + y \to u_r + v_r, \qquad (u_r, v_r) \in G \times G,$$

together with a real number $\Delta E(r) \in \mathbb{R}$ (its EMF score), computed from standard electrode data in the usual way (e.g. $\Delta E = E^\circ_{\text{cathode}} - E^\circ_{\text{anode}}$). We call r spontaneous if $\Delta E(r) > 0$.

Define the set of spontaneous channels and its maximal score by

$$R^+(x, y) := \{\, r \in R(x, y) \mid \Delta E(r) > 0 \,\}, \qquad M(x, y) := \begin{cases} \max\{\Delta E(r) \mid r \in R^+(x, y)\}, & R^+(x, y) \neq \emptyset, \\ 0, & R^+(x, y) = \emptyset. \end{cases}$$

We then define a hyperoperation $\oplus : G \times G \to \mathcal{P}^*(G)$ by

$$x \oplus y := \begin{cases} \{\, u_r, v_r \mid r \in R^+(x, y),\ \Delta E(r) = M(x, y) \,\}, & R^+(x, y) \neq \emptyset, \\ \{x, y\}, & R^+(x, y) = \emptyset, \end{cases}$$

i.e., we collect all product species that occur in at least one spontaneous channel with maximal EMF score; if no spontaneous channel exists, we record "no net reaction" by returning $\{x, y\}$.

Then $(G, \oplus)$ is called a chemical hyperstructure. If $\oplus$ satisfies the classical hypergroup axioms, then $(G, \oplus)$ is a chemical hypergroup. If $\oplus$ is weakly associative and satisfies the reproduction axiom

$$a \oplus G = G = G \oplus a \qquad (\forall a \in G),$$

then $(G, \oplus)$ is a chemical Hv–group. If $\oplus$ is only weakly associative, it is a chemical Hv–semigroup.

Set-extension convention.

Given a hyperoperation $\oplus : G \times G \to \mathcal{P}^*(G)$, we extend it to $\oplus : \mathcal{P}^*(G) \times \mathcal{P}^*(G) \to \mathcal{P}^*(G)$ by

$$A \oplus B := \bigcup_{a \in A,\ b \in B} (a \oplus b), \qquad a \oplus B := \bigcup_{b \in B} (a \oplus b), \qquad A \oplus b := \bigcup_{a \in A} (a \oplus b).$$

This convention is used in weak associativity statements.

Example 3 (Iron redox system (illustrative table))**.** Let

$$G = \{\mathrm{Fe}, \mathrm{Fe}^{2+}, \mathrm{Fe}^{3+}\}.$$

An example of a (commutative) hyperoperation table of the form in Definition 8 is:

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

Whether this $\oplus$ satisfies Hv–semigroup (weak associativity) and/or Hv–group (reproduction) axioms can be checked purely algebraically from the table using the set-extension convention above.

Example 4 (Copper redox system (illustrative table))**.** Let

$$G = \{\mathrm{Cu}, \mathrm{Cu}^{+}, \mathrm{Cu}^{2+}\}.$$

Using standard reduction potentials (for the relevant half-reactions), one may obtain a table of the following form:

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

Again, Hv-type properties are verified by checking the corresponding axioms.

2.4. Weak chemical hyperstructure

A weak chemical hyperstructure is a chemical hyperstructure whose hyperoperation satisfies weak associativity in the sense of Hv–semigroups.

Definition 9 (Weak chemical hyperstructure)**.** Let H be a nonempty set and let $\circ : H \times H \to \mathcal{P}^*(H)$ be a hyperoperation. Extend $\circ$ to nonempty subsets by

$$A \circ B := \bigcup_{a\in A,\, b\in B} (a \circ b), \qquad a \circ B := \bigcup_{b\in B} (a \circ b), \qquad A \circ b := \bigcup_{a\in A} (a \circ b).$$

We say that $(H, \circ)$ is a weak chemical hyperstructure (equivalently, an Hv–semigroup) if it satisfies the weak associativity axiom

$$x \circ (y \circ z) \cap (x \circ y) \circ z \neq \emptyset \qquad (\forall x, y, z \in H),$$

where $y \circ z$ and $x \circ y$ are evaluated in $\mathcal{P}^*(H)$ using the above extension. If, moreover, $x \circ y = y \circ x$ for all $x, y \in H$, then $(H, \circ)$ is called commutative. If instead only $x \circ y \cap y \circ x \neq \emptyset$ holds for all x, y, it is called weakly commutative.

3. Results in this paper

In this section, we present the main results of this paper by formally defining the Weak Superhyperstructure, the Chemical Superhyperstructure, and the Weak Chemical Superhyperstructure.

3.1. Weak superhyperstructure (SHv-Structure)

A weak n-superhyperstructure (also called an SHv-structure) is an Hv-type hyperalgebra carried by the nth iterated powerset: the binary "superhyperoperation" returns a nonempty family of n-level objects and satisfies weak associativity.

Notation.

For any set X, write $\mathcal{P}^*(X) := \mathcal{P}(X) \setminus \{\emptyset\}$. For $n \in \mathbb{N}_0$, let $\mathcal{P}_0(S) := S$ and $\mathcal{P}_{n+1}(S) := \mathcal{P}(\mathcal{P}_n(S))$.

Definition 10 (Set-extension of a superhyperoperation)**.** Let H be a nonempty set and let $\circ : H \times H \to \mathcal{P}^*(H)$ be a hyperoperation. Extend $\circ$ to $\mathcal{P}^*(H)$ by

$$A \circ B := \bigcup_{a\in A,\, b\in B} (a \circ b) \qquad (A, B \in \mathcal{P}^*(H)),$$

and in particular

$$x \circ B := \bigcup_{b\in B} (x \circ b), \qquad A \circ y := \bigcup_{a\in A} (a \circ y) \qquad (x, y \in H,\ A, B \in \mathcal{P}^*(H)).$$

Definition 11 (Weak nth superhyperstructure)**.** Let S be a nonempty set and fix $n \in \mathbb{N}$. A weak n-superhyperstructure (SHv-structure) is a pair

$$(\mathcal{P}_n(S), \circ),$$

where

$$\circ : \mathcal{P}_n(S) \times \mathcal{P}_n(S) \to \mathcal{P}^*(\mathcal{P}_n(S)),$$

is a hyperoperation such that, with the set-extension convention of Definition 10 (applied to $H = \mathcal{P}_n(S)$), the following weak associativity holds:

$$X \circ (Y \circ Z) \cap (X \circ Y) \circ Z \neq \emptyset \qquad (\forall X, Y, Z \in \mathcal{P}_n(S)).$$

If, moreover, the reproduction axiom

$$A \circ \mathcal{P}_n(S) = \mathcal{P}_n(S) = \mathcal{P}_n(S) \circ A \qquad (\forall A \in \mathcal{P}_n(S)),$$

holds (again using the set-extension of $\circ$), then $(\mathcal{P}_n(S), \circ)$ is called an Hv–group on $\mathcal{P}_n(S)$ (or an Hv–group of order n in the superhyperstructure terminology).

Example 5 (A canonical weak n-superhyperstructure via $\cup/\cap$)**.** Let S be any nonempty set and $n \in \mathbb{N}$. Define

$$X \circ Y := \{\, X \cup Y,\ X \cap Y \,\} \qquad (X, Y \in \mathcal{P}_n(S)).$$

Then $X \circ Y \in \mathcal{P}^*(\mathcal{P}_n(S))$ always, and $\circ$ is weakly associative. Indeed, for any X, Y, Z we have

$$X \cup (Y \cup Z) \in X \circ (Y \circ Z) \quad \text{and} \quad (X \cup Y) \cup Z \in (X \circ Y) \circ Z,$$

and these two elements are equal. Hence $X \circ (Y \circ Z) \cap (X \circ Y) \circ Z \neq \emptyset$. On the other hand, $\circ$ is typically not strictly associative because, in general, $X \cap (Y \cup Z) \neq (X \cap Y) \cup Z$ etc. Therefore $(\mathcal{P}_n(S), \circ)$ is a (usually non-strong) weak n-superhyperstructure.

Theorem 1 (Relations to strong superhyperstructures and weak hyperstructures)**.** *1. Let $\star : \mathcal{P}_n(S) \times \mathcal{P}_n(S) \to \mathcal{P}_n(S)$ be a strictly associative (binary) operation. Define the hyperoperation $\circ$ by*

$$X \circ Y := \{\, X \star Y \,\}.$$

Then $(\mathcal{P}_n(S), \circ)$ is a weak n-superhyperstructure.

2. *Let $(H, \cdot)$ be a weak hyperstructure (Hv–semigroup), i.e. $\cdot : H \times H \to \mathcal{P}^*(H)$ is weakly associative. Define $\circ$ on $\mathcal{P}_1(H) = \mathcal{P}(H)$ by the set-extension rule*

$$A \circ B := \bigcup_{a\in A,\, b\in B} (a \cdot b) \qquad (A, B \in \mathcal{P}(H)).$$

Then $(\mathcal{P}(H), \circ)$ is a weak 1-superhyperstructure. Moreover, for singletons,

$$\{x\} \circ \{y\} = x \cdot y \qquad (x, y \in H),$$

so $(H, \cdot)$ is recovered by restricting $\circ$ to singletons.

Proof. (1) Since $\star$ is associative,

$$X \star (Y \star Z) = (X \star Y) \star Z \qquad (\forall X, Y, Z).$$

With $X \circ Y = \{X \star Y\}$, the set-extension yields

$$X \circ (Y \circ Z) = X \circ \{Y \star Z\} = \{X \star (Y \star Z)\},$$

and similarly $(X \circ Y) \circ Z = \{(X \star Y) \star Z\}$. Hence the two sets are equal, in particular they intersect nontrivially.

(2) By construction, for any $A, B \in \mathcal{P}(H)$ the set $A \circ B$ is a union of nonempty sets, hence $A \circ B \in \mathcal{P}^*(H) \subseteq \mathcal{P}(H)$; equivalently, $A \circ B \in \mathcal{P}^*(\mathcal{P}(H))$ when viewed as a subset of $\mathcal{P}(H)$. Weak associativity of $\circ$ on $\mathcal{P}(H)$ follows from weak associativity of $\cdot$ by a standard "element-chasing" argument using Definition 10. Finally, $\{x\} \circ \{y\} = x \cdot y$ is immediate from the definition. □

Theorem 2 (Induced weak n-superhyperstructure on closed subsets)**.** *Let $(\mathcal{P}_n(S), \circ)$ be a weak n-superhyperstructure and let $U \subseteq \mathcal{P}_n(S)$ be nonempty. Assume U is closed under $\circ$, i.e.*

$$X, Y \in U \implies X \circ Y \subseteq U.$$

Then, with the restricted hyperoperation $\circ|_{U \times U}$, the pair $(U, \circ)$ is a weak hyperstructure (Hv–semigroup).

Proof. For $X, Y \in U$, we have $X \circ Y \in \mathcal{P}^*(\mathcal{P}_n(S))$ by definition of the ambient structure. Closure implies $X \circ Y \subseteq U$, hence $X \circ Y \in \mathcal{P}^*(U)$, so $\circ : U \times U \to \mathcal{P}^*(U)$. Weak associativity on U follows by applying weak associativity in $\mathcal{P}_n(S)$ to any $X, Y, Z \in U$ and using that all intermediate products remain in U by closure. □

Definition 12 (Homomorphism of weak n-superhyperstructures)**.** Let $(\mathcal{P}_n(S), \circ_S)$ and $(\mathcal{P}_m(T), \circ_T)$ be weak superhyperstructures. For a map $\varphi : \mathcal{P}_n(S) \to \mathcal{P}_m(T)$, define its direct image on subsets by

$$\varphi^*(A) := \{\varphi(a) \mid a \in A\} \qquad (A \in \mathcal{P}^*(\mathcal{P}_n(S))).$$

We call φ a homomorphism if for all $X, Y \in \mathcal{P}_n(S)$,

$$\varphi^*(X \circ_S Y) \subseteq \varphi(X) \circ_T \varphi(Y).$$

Theorem 3 (Homomorphic image as a sub–SHv-structure under closure)**.** *Let $\varphi : (\mathcal{P}_n(S), \circ_S) \to (\mathcal{P}_m(T), \circ_T)$ be a surjective homomorphism and set $V := \varphi(\mathcal{P}_n(S)) \subseteq \mathcal{P}_m(T)$. Assume in addition that V is closed under $\circ_T$, i.e.*

$$U_1, U_2 \in V \implies U_1 \circ_T U_2 \subseteq V.$$

Then $(V, \circ_T)$ is a weak m-superhyperstructure (the restriction of the target SHv-structure to V).

Proof. Since $\circ_T$ is weakly associative on $\mathcal{P}_m(T)$, it remains weakly associative on V once we know it is well-typed there. Closure ensures $U_1 \circ_T U_2 \subseteq V$, and nonemptiness of $U_1 \circ_T U_2$ is inherited from the ambient codomain $\mathcal{P}^*(\mathcal{P}_m(T))$. Hence $\circ_T : V \times V \to \mathcal{P}^*(V)$ and weak associativity holds on V by restriction. □

Theorem 4 (Deterministic regime implies full associativity)**.** *Let $(\mathcal{P}_n(S), \circ)$ be a weak n-superhyperstructure. Assume $\circ$ is single-valued in the sense that*

$$|X \circ Y| = 1 \qquad (\forall X, Y \in \mathcal{P}_n(S)).$$

Then $\circ$ is strictly associative:

$$X \circ (Y \circ Z) = (X \circ Y) \circ Z \qquad (\forall X, Y, Z \in \mathcal{P}_n(S)),$$

and consequently every fully parenthesized evaluation of $X_1 \circ \cdots \circ X_k$ yields the same singleton subset of $\mathcal{P}_n(S)$.

Proof. For X, Y, Z, both $X \circ (Y \circ Z)$ and $(X \circ Y) \circ Z$ are singletons (because $Y \circ Z$ and $X \circ Y$ are singletons, and we use the set-extension). Weak associativity gives that these two singletons have nonempty intersection, hence they are equal, proving strict associativity for triples. The statement for longer products follows by induction on k, since strict associativity makes the value independent of parenthesization. □

3.2. Chemical superhyperstructure

A Chemical Superhyperstructure of order n encodes hierarchical (powerset–iterated) redox interactions by selecting "major" product modules according to a maximal EMF score.

Definition 13 (Chemical Superhyperstructure of order n)**.** Let G be a finite nonempty set of chemical species (e.g., oxidation states, ions, molecules). For $n \in \mathbb{N}$, let $\mathcal{P}_n(G)$ denote the nth iterated powerset (Definition 1) and write

$$\mathcal{P}^*(\mathcal{P}_n(G)) := \mathcal{P}(\mathcal{P}_n(G)) \setminus \{\emptyset\}.$$

Assume that for each $n \geq 1$ and each ordered pair $(A, B) \in \mathcal{P}_n(G) \times \mathcal{P}_n(G)$ we are given

1. a nonempty set of admissible redox channels

$$\Gamma_n(A, B) \subseteq \mathcal{P}_{n-1}(G) \times \mathcal{P}_{n-1}(G), \qquad \Gamma_n(A, B) \neq \emptyset,$$

whose elements $(Y, Z) \in \Gamma_n(A, B)$ are interpreted as possible product-module pairs for the interaction of A and B; and
2. an EMF score (cell-potential score)

$$\Delta E_n(A, B; \cdot, \cdot) : \Gamma_n(A, B) \to \mathbb{R}.$$

Define the set of maximizers (argmax set)

$$\mathrm{Max}_n(A, B) := \Big\{ (Y, Z) \in \Gamma_n(A, B) \;\Big|\; \Delta E_n(A, B; Y, Z) = \max_{(Y', Z') \in \Gamma_n(A,B)} \Delta E_n(A, B; Y', Z') \Big\}.$$

Define the major (positive) maximizers

$$\mathrm{Max}_n^+(A, B) := \Big\{ (Y, Z) \in \mathrm{Max}_n(A, B) \;\Big|\; \Delta E_n(A, B; Y, Z) > 0 \Big\}.$$

Now define a superhyperoperation

$$\oplus^{(n)} : \mathcal{P}_n(G) \times \mathcal{P}_n(G) \to \mathcal{P}^*(\mathcal{P}_n(G)),$$

by the rule

$$A \oplus^{(n)} B := \Big\{ \{Y, Z\} \in \mathcal{P}_n(G) \;\Big|\; (Y, Z) \in \mathrm{Max}_n^+(A, B) \Big\},$$

if $\mathrm{Max}_n^+(A, B) \neq \emptyset$, and otherwise (if no positive channel exists) by

$$A \oplus^{(n)} B := \Big\{ \{Y, Z\} \in \mathcal{P}_n(G) \;\Big|\; (Y, Z) \in \mathrm{Max}_n(A, B) \Big\}.$$

Then $(\mathcal{P}_n(G), \oplus^{(n)})$ is called a Chemical Superhyperstructure of order n.

Remark 1 (Chemical interpretation beyond the first level)**.** For $n \geq 2$, elements of $\mathcal{P}_n(G)$ are collections of lower-level species-sets. In applications, one may interpret them as modules/complexes (e.g., grouped redox moieties or coarse-grained ensembles). Accordingly, a selected product $\{Y, Z\} \subseteq \mathcal{P}_{n-1}(G)$ should be read as a pair of alternative product modules; at higher levels the construction is a controlled symbolic abstraction unless additional stoichiometric/kinetic constraints are imposed.

Theorem 5 (Reference-electrode (additive gauge) invariance)**.** *Assume the EMF scores ΔE_n are computed from assigned standard potentials $E^\circ : G \to \mathbb{R}$ only through potential differences (e.g., $E^\circ_{cathode} - E^\circ_{anode}$ for each channel), so that adding a constant to all E° values does not change any score. Let $c \in \mathbb{R}$ and define*

$$\widetilde{E}^\circ(x) := E^\circ(x) + c \quad \text{for } x \in G.$$

Let $\oplus^{(n)}_{E^\circ}$ and $\oplus^{(n)}_{\widetilde{E}^\circ}$ be the induced superhyperoperations. Then

$$A \oplus^{(n)}_{E^\circ} B = A \oplus^{(n)}_{\widetilde{E}^\circ} B \qquad (\forall A, B \in \mathcal{P}_n(G)).$$

Proof. All channel scores $\Delta E_n(A, B; Y, Z)$ are unchanged under $E^\circ \mapsto \widetilde{E}^\circ$ because additive constants cancel in differences. Hence $\Gamma_n(A, B)$, the maximal value, and the argmax sets $\mathrm{Max}_n(A, B)$ and $\mathrm{Max}^+_n(A, B)$ are unchanged. Therefore the selected product-sets coincide. □

Example 6 (Order 2: metal–ion displacement (well-typed version))**.** Let

$$G = \{\mathrm{Zn}, \mathrm{Zn}^{2+}, \mathrm{Cu}, \mathrm{Cu}^{2+}, \mathrm{Ag}, \mathrm{Ag}^{+}\}.$$

Fix standard reduction potentials (in volts)

$$E^\circ(\mathrm{Zn}^{2+}/\mathrm{Zn}) = -0.76, \qquad E^\circ(\mathrm{Cu}^{2+}/\mathrm{Cu}) = +0.34, \qquad E^\circ(\mathrm{Ag}^{+}/\mathrm{Ag}) = +0.80.$$

Let $A = \big\{\{\mathrm{Zn}\}, \{\mathrm{Zn}^{2+}\}\big\} \in \mathcal{P}_2(G)$ and $B = \big\{\{\mathrm{Ag}^{+}\}, \{\mathrm{Cu}^{2+}\}\big\} \in \mathcal{P}_2(G)$. Consider displacement channels of the form

$$\mathrm{M} + \mathrm{N}^{q+} \to \mathrm{M}^{p+} + \mathrm{N},$$

and score each channel by $\Delta E = E^\circ_{\mathrm{cathode}} - E^\circ_{\mathrm{anode}}$. Then the candidates include

$$\mathrm{Zn} + \mathrm{Ag}^{+} \to \mathrm{Zn}^{2+} + \mathrm{Ag}, \qquad \Delta E = 0.80 - (-0.76) = 1.56,$$

$$\mathrm{Zn} + \mathrm{Cu}^{2+} \to \mathrm{Zn}^{2+} + \mathrm{Cu}, \qquad \Delta E = 0.34 - (-0.76) = 1.10.$$

Thus the (positive) maximizer is the $\mathrm{Zn}/\mathrm{Ag}^{+}$ channel, and hence

$$A \oplus^{(2)} B = \Big\{\big\{\{\mathrm{Zn}^{2+}\}, \{\mathrm{Ag}\}\big\}\Big\} \subseteq \mathcal{P}_2(G).$$

Theorem 6 (Underlying n-superhyperstructure)**.** *For each $n \geq 1$, the pair $(\mathcal{P}_n(G), \oplus^{(n)})$ is an nth superhyperstructure in the sense that*

$$\oplus^{(n)} : \mathcal{P}_n(G) \times \mathcal{P}_n(G) \to \mathcal{P}^*(\mathcal{P}_n(G)),$$

is a well-defined (everywhere-defined) superhyperoperation. No associativity or reproduction axiom is asserted unless imposed separately.

Proof. By Definition 13, for any $A, B \in \mathcal{P}_n(G)$ the set $\Gamma_n(A, B)$ is nonempty, so $\mathrm{Max}_n(A, B) \neq \emptyset$. By construction, $A \oplus^{(n)} B$ is a nonempty collection of sets of the form $\{Y, Z\}$ with $Y, Z \in \mathcal{P}_{n-1}(G)$, hence $\{Y, Z\} \in \mathcal{P}_n(G)$ and $A \oplus^{(n)} B \in \mathcal{P}^*(\mathcal{P}_n(G))$. □

Theorem 7 (Reduction to chemical hyperstructure at $n = 1$)**.** *Let $n = 1$. Identify each $x \in G$ with the singleton $\{x\} \in \mathcal{P}_1(G) = \mathcal{P}(G)$. Define an induced hyperoperation on G by*

$$x \oplus y := \{\, u \in G \mid \{u\} \in U \text{ for some } U \in \{\{x\}\} \oplus^{(1)} \{\{y\}\} \,\}.$$

Then $(G, \oplus)$ is a chemical hyperstructure induced from the order-1 chemical superhyperstructure by restriction to singletons.

Proof. Let $n = 1$. Then $\mathcal{P}_1(G) = \mathcal{P}(G)$ and $\mathcal{P}_0(G) = G$. Embed G into $\mathcal{P}(G)$ by $i(x) := \{x\}$. By the definition of the order-1 superhyperoperation, for $x, y \in G$ we have

$$\{x\} \oplus^{(1)} \{y\} \subseteq \mathcal{P}^*(\mathcal{P}(G)),$$

and each $U \in \{x\} \oplus^{(1)} \{y\}$ is a (nonempty) subset of G consisting of those major products selected by the maximal positive EMF rule for the redox input $x + y$. Define the induced hyperoperation on G by

$$x \oplus y := \bigcup_{U \in \{x\} \oplus^{(1)} \{y\}} U = \{\, u \in G \mid u \in U \text{ for some } U \in \{x\} \oplus^{(1)} \{y\} \,\}.$$

Then $x \oplus y$ is exactly the set of major products of the reaction channel(s) $x + y \to \cdots$ chosen by maximal positive EMF, i.e., $(G, \oplus)$ is precisely the chemical hyperstructure obtained by restricting the order-1 chemical superhyperstructure to singletons. □

Theorem 8 (Commutativity under symmetric channel data)**.** *Assume that for all $n \geq 1$ and all $A, B \in \mathcal{P}_n(G)$:*

$$(Y, Z) \in \Gamma_n(A, B) \iff (Z, Y) \in \Gamma_n(B, A),$$

and

$$\Delta E_n(A, B; Y, Z) = \Delta E_n(B, A; Z, Y).$$

Then $A \oplus^{(n)} B = B \oplus^{(n)} A$ for all $A, B \in \mathcal{P}_n(G)$.

Proof. The assumptions imply that $\Gamma_n(A, B)$ and $\Gamma_n(B, A)$ correspond by swapping coordinates, preserving scores. Hence $\mathrm{Max}_n(A, B)$ and $\mathrm{Max}_n(B, A)$ (and their positive parts) correspond, yielding identical selected unordered pairs $\{Y, Z\}$. □

Theorem 9 (Induced sub–superhyperstructure)**.** *Let $(\mathcal{P}_n(G), \oplus^{(n)})$ be a chemical superhyperstructure. If $\emptyset \neq U \subseteq \mathcal{P}_n(G)$ satisfies the closure condition*

$$A, B \in U \implies A \oplus^{(n)} B \subseteq U,$$

then $(U, \oplus^{(n)})$ is again a chemical superhyperstructure of order n.

Proof. Closure implies $\oplus^{(n)} : U \times U \to \mathcal{P}^*(U)$, and the defining maximization rule is unchanged under restriction to U. □

Theorem 10 (Species–permutation automorphisms)**.** *Let $\sigma : G \to G$ be a bijection. Extend it recursively to $\sigma^{[0]} = \sigma$ and*

$$\sigma^{[k+1]}(X) := \{\sigma^{[k]}(x) : x \in X\} \qquad (X \in \mathcal{P}_{k+1}(G)),$$

and write $\sigma^{(n)} := \sigma^{[n]} : \mathcal{P}_n(G) \to \mathcal{P}_n(G)$. Assume the channel data are equivariant:

$$(Y, Z) \in \Gamma_n(A, B) \iff (\sigma^{(n-1)}(Y), \sigma^{(n-1)}(Z)) \in \Gamma_n(\sigma^{(n)}(A), \sigma^{(n)}(B)),$$

and the scores are preserved:

$$\Delta E_n(\sigma^{(n)}(A), \sigma^{(n)}(B); \sigma^{(n-1)}(Y), \sigma^{(n-1)}(Z)) = \Delta E_n(A, B; Y, Z).$$

Then $\sigma^{(n)}$ is an automorphism of the chemical superhyperstructure:

$$\sigma^{(n)}(A \oplus^{(n)} B) = \sigma^{(n)}(A) \oplus^{(n)} \sigma^{(n)}(B) \qquad (\forall A, B \in \mathcal{P}_n(G)),$$

where for a subset $U \subseteq \mathcal{P}_n(G)$ we write $\sigma^{(n)}(U) = \{\sigma^{(n)}(u) : u \in U\}$.

Proof. Since $\sigma : G \to G$ is a bijection, each extension $\sigma^{(n)} : \mathcal{P}_n(G) \to \mathcal{P}_n(G)$ is a bijection. Fix $A, B \in \mathcal{P}_n(G)$ and let $U \in A \oplus^{(n)} B$. By definition, $U = \{Y, Z\}$ for some $(Y, Z) \in \Gamma_n(A, B)$ that attains the maximal EMF score (and, if applicable, is among the positive maximizers). By channel equivariance, $(\sigma^{(n-1)}(Y), \sigma^{(n-1)}(Z)) \in$

$\Gamma_n(\sigma^{(n)}(A), \sigma^{(n)}(B))$, and by score preservation it has the same EMF value, hence it is again a maximizer (and positivity is preserved). Therefore $\{\sigma^{(n-1)}(Y), \sigma^{(n-1)}(Z)\} \in \sigma^{(n)}(A) \oplus^{(n)} \sigma^{(n)}(B)$, i.e.,

$$\sigma^{(n)}(A \oplus^{(n)} B) \subseteq \sigma^{(n)}(A) \oplus^{(n)} \sigma^{(n)}(B).$$

Applying the same argument to σ^{-1} yields the reverse inclusion, hence equality. □

3.3. Weak nth chemical superhyperstructure

A weak n-chemical superhyperstructure is a weak n-superhyperstructure whose superhyperoperation is induced by a "maximal positive EMF" (major-product) selection rule.

Notation.

For a set X, write $\mathcal{P}^*(X) := \mathcal{P}(X) \setminus \{\emptyset\}$. Fix $n \geq 1$. We use the iterated powerset convention $\mathcal{P}_0(G) = G$ and $\mathcal{P}_{k+1}(G) = \mathcal{P}(\mathcal{P}_k(G))$ for $k \geq 0$. Thus $\mathcal{P}_n(G)$ is the n-th powerset and $\mathcal{P}^*(\mathcal{P}_n(G)) = \mathcal{P}(\mathcal{P}_n(G)) \setminus \{\emptyset\}$.

Definition 14 (Weak nth Chemical Superhyperstructure)**.** Let G be a finite set (interpreted as chemical species, oxidation states, etc.). Assume we are given, for each $A, B \in \mathcal{P}_n(G)$,

- a nonempty set of admissible product-channels

$$\Gamma_n(A, B) \subseteq \mathcal{P}_{n-1}(G) \times \mathcal{P}_{n-1}(G),$$

- and a score function (EMF score)

$$\Delta E_n(A, B; \cdot, \cdot) : \Gamma_n(A, B) \to \mathbb{R}.$$

Define the set of positive maximizers

$$\begin{aligned} {}^{+}\mathrm{Argmax}\, \Delta E_n(A, B) :=& \Big\{ (Y, Z) \in \Gamma_n(A, B) \;\Big|\; \Delta E_n(A, B; Y, Z) \\ &= \max_{\substack{(Y', Z') \in \Gamma_n(A,B) \\ \Delta E_n(A,B;Y',Z') > 0}} \Delta E_n(A, B; Y', Z'),\ \Delta E_n(A, B; Y, Z) > 0 \Big\}. \end{aligned}$$

(We assume this set is nonempty for every A, B; otherwise one may allow $\emptyset$ in the codomain.)
Now define a superhyperoperation

$$\oplus^{(n)} : \mathcal{P}_n(G) \times \mathcal{P}_n(G) \to \mathcal{P}^*(\mathcal{P}_n(G)),$$

by

$$A \oplus^{(n)} B := \Big\{ \{Y, Z\} \in \mathcal{P}_n(G) \;\Big|\; (Y, Z) \in {}^{+}\mathrm{Argmax}\, \Delta E_n(A, B) \Big\}.$$

(Here $\{Y, Z\}$ is the unordered subset of $\mathcal{P}_{n-1}(G)$, hence an element of $\mathcal{P}(\mathcal{P}_{n-1}(G)) = \mathcal{P}_n(G)$.)

Set-extension (for bracketing).

For any $U \subseteq \mathcal{P}_n(G)$ and $A \in \mathcal{P}_n(G)$, set

$$A \oplus^{(n)} U := \bigcup_{u \in U} (A \oplus^{(n)} u), \qquad U \oplus^{(n)} A := \bigcup_{u \in U} (u \oplus^{(n)} A).$$

We call $(\mathcal{P}_n(G), \oplus^{(n)})$ a weak n-chemical superhyperstructure if

$$X \oplus^{(n)} (Y \oplus^{(n)} Z) \cap (X \oplus^{(n)} Y) \oplus^{(n)} Z \neq \emptyset \qquad (\forall X, Y, Z \in \mathcal{P}_n(G)),$$

where the expressions are interpreted via the set-extension above.

We say it is commutative if $A \oplus^{(n)} B = B \oplus^{(n)} A$ for all A, B. (If one only requires $A \oplus^{(n)} B \cap B \oplus^{(n)} A \neq \emptyset$, one may call it weakly commutative.)

Theorem 11 (EMF-deterministic regime implies strict associativity)**.** *Let* $(\mathcal{P}_n(G), \oplus^{(n)})$ *be a weak n- chemical superhyperstructure. Assume that every binary product is singleton-valued:*

$$\left|A \oplus^{(n)} B\right| = 1 \qquad (\forall A, B \in \mathcal{P}_n(G)).$$

Then $\oplus^{(n)}$ *is strictly associative:*

$$X \oplus^{(n)} (Y \oplus^{(n)} Z) = (X \oplus^{(n)} Y) \oplus^{(n)} Z \qquad (\forall X, Y, Z \in \mathcal{P}_n(G)).$$

Proof. By weak associativity, $X \oplus^{(n)} (Y \oplus^{(n)} Z) \cap (X \oplus^{(n)} Y) \oplus^{(n)} Z \neq \emptyset$. Since $|Y \oplus^{(n)} Z| = 1$, the set-extension gives $X \oplus^{(n)} (Y \oplus^{(n)} Z) = X \oplus^{(n)} U$ for a unique $U \in \mathcal{P}_n(G)$, hence is a singleton (by the hypothesis $|\cdot \oplus^{(n)} \cdot| = 1$); similarly the other bracketing is a singleton. Two singleton sets with nonempty intersection must be equal. □

Example 7 (Weak 2-chemical superhyperstructure: Zn–Cu–Fe system)**.** Let

$$G = \{\mathrm{Zn}, \mathrm{Zn}^{2+}, \mathrm{Cu}, \mathrm{Cu}^{2+}, \mathrm{Fe}, \mathrm{Fe}^{2+}\},$$

with standard reduction potentials $E^\circ(\mathrm{Zn}^{2+}/\mathrm{Zn}) = -0.76$, $E^\circ(\mathrm{Cu}^{2+}/\mathrm{Cu}) = +0.34$, $E^\circ(\mathrm{Fe}^{2+}/\mathrm{Fe}) = -0.44$ (V). Note that $\mathcal{P}_1(G) = \mathcal{P}(G)$ contains all subsets; we will use singletons to represent individual species. Consider the elements of $\mathcal{P}_2(G) = \mathcal{P}(\mathcal{P}(G))$:

$$A = \big\{\{\mathrm{Zn}\}, \{\mathrm{Fe}\}\big\}, \quad B = \big\{\{\mathrm{Cu}^{2+}\}, \{\mathrm{Zn}^{2+}\}\big\}, \quad C = \big\{\{\mathrm{Fe}^{2+}\}, \{\mathrm{Zn}\}\big\}.$$

Assume the channel/score data $(\Gamma_2, \Delta E_2)$ encode the usual displacement reactions and EMF, so that the maximal positive EMF among pairs $a \in A$, $b \in B$ is attained for $\mathrm{Zn} + \mathrm{Cu}^{2+} \to \mathrm{Zn}^{2+} + \mathrm{Cu}$ with $\Delta E = 0.34 - (-0.76) = 1.10$ V. Then

$$A \oplus^{(2)} B = \Big\{\big\{\{\mathrm{Zn}^{2+}\}, \{\mathrm{Cu}\}\big\}\Big\}.$$

Similarly, the maximal positive EMF among pairs $b \in B$, $c \in C$ is attained for $\mathrm{Cu}^{2+} + \mathrm{Zn} \to \mathrm{Cu} + \mathrm{Zn}^{2+}$ with the same EMF, hence

$$B \oplus^{(2)} C = \Big\{\big\{\{\mathrm{Zn}^{2+}\}, \{\mathrm{Cu}\}\big\}\Big\}.$$

Let $U := \big\{\{\mathrm{Zn}^{2+}\}, \{\mathrm{Cu}\}\big\} \in \mathcal{P}_2(G)$. Then $B \oplus^{(2)} C = \{U\}$, so by set-extension

$$A \oplus^{(2)} (B \oplus^{(2)} C) = A \oplus^{(2)} \{U\} = A \oplus^{(2)} U = \{U\},$$

and similarly $(A \oplus^{(2)} B) \oplus^{(2)} C = \{U\}$. Hence the weak associativity intersection is nonempty.

Example 8 (Weak 1-chemical superhyperstructure: Ce–Fe system)**.** Let $G = \{\mathrm{Ce}^{4+}, \mathrm{Ce}^{3+}, \mathrm{Fe}^{2+}, \mathrm{Fe}^{3+}\}$ with $E^\circ(\mathrm{Ce}^{4+}/\mathrm{Ce}^{3+}) = 1.61$ V and $E^\circ(\mathrm{Fe}^{3+}/\mathrm{Fe}^{2+}) = 0.77$ V. Take

$$A = \{\mathrm{Ce}^{4+}, \mathrm{Fe}^{2+}\}, \quad B = \{\mathrm{Ce}^{3+}, \mathrm{Fe}^{3+}\}, \quad C = \{\mathrm{Ce}^{3+}, \mathrm{Fe}^{3+}\} \in \mathcal{P}_1(G) = \mathcal{P}(G).$$

Assume the data $(\Gamma_1, \Delta E_1)$ select the unique spontaneous channel $\mathrm{Ce}^{4+} + \mathrm{Fe}^{2+} \to \mathrm{Ce}^{3+} + \mathrm{Fe}^{3+}$ with EMF 0.84 V, so

$$A \oplus^{(1)} B = \big\{\{\mathrm{Ce}^{3+}, \mathrm{Fe}^{3+}\}\big\}.$$

Let $P := \{\mathrm{Ce}^{3+}, \mathrm{Fe}^{3+}\}$. Then $B \oplus^{(1)} C = \{P\}$ and by set-extension $A \oplus^{(1)} (B \oplus^{(1)} C) = A \oplus^{(1)} P = \{P\}$, and likewise $(A \oplus^{(1)} B) \oplus^{(1)} C = \{P\}$.

Theorem 12 (Weak n-chemical superhyperstructures are weak n-superhyperstructures)**.** *If* $(\mathcal{P}_n(G), \oplus^{(n)})$ *is a weak n-chemical superhyperstructure, then it is a weak n-superhyperstructure in the sense of Definition 11.*

Proof. By definition, $\oplus^{(n)} : \mathcal{P}_n(G) \times \mathcal{P}_n(G) \to \mathcal{P}^*(\mathcal{P}_n(G))$, so the operation is well-typed with nonempty values. The required weak associativity $X \oplus^{(n)} (Y \oplus^{(n)} Z) \cap (X \oplus^{(n)} Y) \oplus^{(n)} Z \neq \emptyset$ is exactly the defining axiom. □

Theorem 13 (Restriction to singletons at $n = 1$)**.** *Let $n = 1$ and identify each $x \in G$ with $\{x\} \in \mathcal{P}_1(G) = \mathcal{P}(G)$. Define a hyperoperation $\circ$ on G by*

$$x \circ y := \{\, u \in G \mid u \in U \text{ for some } U \in \{\{x\}\} \oplus^{(1)} \{\{y\}\} \,\}.$$

Then $(G, \circ)$ is a weak chemical hyperstructure induced from $(\mathcal{P}_1(G), \oplus^{(1)})$.

Proof. The definition of $\circ$ is precisely the restriction of $\oplus^{(1)}$ to singleton inputs, unpacking the fact that $\oplus^{(1)}$ returns a family of product-subsets of G. Weak associativity of $\oplus^{(1)}$ on $\mathcal{P}(G)$, together with the set-extension convention, implies the Hv-type weak associativity for $\circ$ on G. □

Theorem 14 (Induced sub–weak chemical superhyperstructure)**.** *Let $(\mathcal{P}_n(G), \oplus^{(n)})$ be a weak n-chemical superhyperstructure and let $\emptyset \neq U \subseteq \mathcal{P}_n(G)$ satisfy*

$$A, B \in U \implies A \oplus^{(n)} B \subseteq U.$$

Then $(U, \oplus^{(n)}|_{U \times U})$ is a weak n-chemical superhyperstructure.

Proof. Closure ensures $\oplus^{(n)} : U \times U \to \mathcal{P}^*(U)$. Moreover, if $X, Y, Z \in U$, then $Y \oplus^{(n)} Z \subseteq U$ and by set-extension $X \oplus^{(n)} (Y \oplus^{(n)} Z) \subseteq U$ and $(X \oplus^{(n)} Y) \oplus^{(n)} Z \subseteq U$. The weak associativity intersection is nonempty in $\mathcal{P}_n(G)$, hence also nonempty in U. □

Theorem 15 (Species–permutation automorphisms)**.** *Let $\sigma : G \to G$ be a bijection and extend it to $\sigma^{(n)} : \mathcal{P}_n(G) \to \mathcal{P}_n(G)$ by $\sigma^{(0)} = \sigma$ and $\sigma^{(k+1)}(X) = \{\sigma^{(k)}(x) : x \in X\}$. Assume the channel/score data are σ-equivariant, i.e. for all $A, B \in \mathcal{P}_n(G)$ and $(Y, Z) \in \mathcal{P}_{n-1}(G) \times \mathcal{P}_{n-1}(G)$,*

$$(Y, Z) \in \Gamma_n(A, B) \iff (\sigma^{(n-1)}(Y), \sigma^{(n-1)}(Z)) \in \Gamma_n(\sigma^{(n)}(A), \sigma^{(n)}(B)),$$

and the scores are preserved:

$$\Delta E_n(\sigma^{(n)}(A), \sigma^{(n)}(B); \sigma^{(n-1)}(Y), \sigma^{(n-1)}(Z)) = \Delta E_n(A, B; Y, Z).$$

Then $\sigma^{(n)}$ is an automorphism:

$$\sigma^{(n)}(A \oplus^{(n)} B) = \sigma^{(n)}(A) \oplus^{(n)} \sigma^{(n)}(B) \qquad (\forall A, B \in \mathcal{P}_n(G)).$$

Proof. Equivariance gives a bijection between admissible channels for (A, B) and for $(\sigma^{(n)}(A), \sigma^{(n)}(B))$, and score preservation implies that ${}^{+}\mathrm{Argmax}\, \Delta E_n(A, B)$ is mapped onto ${}^{+}\mathrm{Argmax}\, \Delta E_n(\sigma^{(n)}(A), \sigma^{(n)}(B))$. Therefore the selected product-elements $\{Y, Z\}$ are carried exactly to the selected product-elements $\{\sigma^{(n-1)}(Y), \sigma^{(n-1)}(Z)\}$, which is precisely the displayed identity. □

Theorem 16 (Commutativity under symmetric channel data)**.** *Assume that for all $A, B \in \mathcal{P}_n(G)$ the channel data and scores are symmetric in the sense that*

$$(Y, Z) \in \Gamma_n(A, B) \iff (Z, Y) \in \Gamma_n(B, A), \qquad \Delta E_n(A, B; Y, Z) = \Delta E_n(B, A; Z, Y).$$

Then $A \oplus^{(n)} B = B \oplus^{(n)} A$ for all $A, B \in \mathcal{P}_n(G)$.

Proof. The symmetry assumptions identify the positive maximizers for (A, B) with those for (B, A) via $(Y, Z) \leftrightarrow (Z, Y)$, hence the induced sets of selected unordered products $\{Y, Z\}$ coincide. □

4. Conclusion and future work

In this paper, we introduced the notion of the Chemical Superhyperstructure and examined its foundational properties. We also proposed the concept of a Weak Chemical Superhyperstructure within the framework of Weak Superhyperstructures and provided an initial exploration of its structural behavior. Our superhyper- structural operations admit a formal network interpretation: each evaluation selects product multisets, yielding directed hyperedges (reaction rules) and an equivalent Petri-net incidence representation.

For future research, we aim to:

- apply these hyperstructural models to a wide range of chemical systems and reaction networks;
- extend the framework through integration with uncertainty-based models, such as Fuzzy Sets [21], Intuitionistic Fuzzy Sets [22], Neutrosophic Sets [23], Hyper Uncertain Sets [24], Uncertain Sets [25,26], and Plithogenic Sets [27,28];
- investigate connections with hypergraph [29–31] and superhypergraph structures [32], as well as the recently proposed molecular superhypergraph model [33].

These directions promise to deepen our understanding of hierarchical, nonlinear, and uncertain relationships that govern complex chemical phenomena.

Disclaimer

This work presents theoretical concepts that have not yet undergone practical testing or validation. Future researchers are encouraged to apply and assess these ideas in empirical contexts. While every effort has been made to ensure accuracy and appropriate referencing, unintentional errors or omissions may still exist. Readers are advised to verify referenced materials on their own. The views and conclusions expressed here are the authors' own and do not necessarily reflect those of their affiliated organizations.

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