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Hyperstructures and superhyperstructures for Hierarchical biochemical, electrochemical, geochemical, photochemical, radiochemical, medicinal-chemical, and neurochemical systems

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Abstract: Set-valued operations are useful when one input state admits several chemically distinct outcomes, but an ordinary powerset does not distinguish alternative outcomes from co-products and does not preserve stoichiometric multiplicity. This paper develops a type-consistent framework in which atomic species generate a free commutative multiset monoid, elementary hyperoperations return nonempty sets of product multisets, and (m, n)-superhyperoperations act between explicitly defined iterated nonempty powersets. Domain-specific feasibility predicates impose balance, energetic, kinetic, and selection constraints without changing the common algebraic type. Two general results are established: elementary balance is preserved along every finite admissible path, and the $(0, 1)$ construction reduces exactly to the underlying hyperoperation. The framework is specialized to biochemical, geochemical, photochemical, electrochemical, radiochemical, neurochemical, and medicinal-chemical systems. Machine-checkable stoichiometric residuals are reported for representative channels. The quantitative checks include the Daniell-cell value $E^{\circ}_{\mathrm{cell}} = 1.103\,\mathrm{V}$, the photon energy $hc/(365\,\mathrm{nm}) = 3.3968\,\mathrm{eV}$, and evaluated ^{212}Bi branching fractions of 64.06% and 35.94%, which sum to 100.00%. These checks validate the internal consistency of the formal examples; they are not presented as new laboratory measurements.

Keywords: hyperoperation, superhyperstructure, reaction multiset, stoichiometric validation, hierarchical chemical system, set-valued dynamics

1. Introduction

Classical operations return one output for each admissible input. Chemical and biological systems frequently require a different semantics: one reactant state may admit several alternative channels, while each channel may contain several co-products with nonunit stoichiometric coefficients. Hyperstructure theory supplies the first part of this semantics by replacing a single-valued operation with a set-valued operation [1–3]. Reaction-network, Petri-net, and rule-based methods supply complementary descriptions of multiplicity, reachability, and composition [4,5]. A chemically usable hyperstructure should therefore distinguish three objects:

1. an atomic state, such as a species, surface microstate, or nuclide;
2. a multiset of jointly present reactants or products; and
3. a set of alternative product multisets.

Earlier chemical-hyperstructure formulations select products using redox criteria [6–8]. The central difficulty in extending this idea to nested or hierarchical systems is not merely to apply the powerset operator, but to keep every level well typed and to retain chemically necessary multiplicities. The present formulation addresses that difficulty by using the free commutative multiset monoid as the state space on which hyperoperations act. Iterated nonempty powersets are then applied to that state space, not directly to an ambiguous mixture of species and product sets. Classical structures, hyperstructures, superhyperstructures, and (m, n)-superhyperstructures are presented in Table 1.

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

Structure type	Underlying input level	Operation signature
Classical structure	H	$f : H^r \to H$
Hyperstructure	H	$h : D \subseteq H^r \to \mathcal{P}_*(H)$
n-superhyperstructure	$\mathcal{P}_*^n(H)$	$F : D_n \subseteq (\mathcal{P}_*^n(H))^r \to \mathcal{P}_*^n(H)$
(m,n)-superhyperstructure	input level $\mathcal{P}_*^m(H)$, output level $\mathcal{P}_*^n(H)$	$F^{(m,n)} : D^{(m)} \subseteq (\mathcal{P}_*^m(H))^r \to \mathcal{P}_*^n(H)$

The research question is: *Can one common, type-consistent algebraic construction represent alternative reaction channels, joint products with multiplicity, and hierarchies of pathway families while preserving domain-specific balance constraints?* The paper answers this question affirmatively under explicit assumptions. Its contributions are:

1. a separation of atomic states, reaction multisets, alternative channels, and iterated pathway families;
2. a single definition of an (m,n)-superhyperoperation in which m is the input powerset level, n is the output powerset level, and r is the arity;
3. a proof that additive balance residuals remain admissible along finite paths;
4. domain specializations whose feasibility data are part of the mathematical object rather than unspecified narrative conditions; and
5. exact, reproducible arithmetic checks for representative biochemical, geochemical, photochemical, electrochemical, radiochemical, neurochemical, and medicinal-chemical channels.

The scope is theoretical. The numerical values used below are evaluated constants or direct consequences of balanced equations; no new experiment, patient data, animal data, or molecular simulation is claimed. This distinction avoids treating internal consistency checks as experimental validation.

2. Preliminaries

Throughout, an atomic set may be finite or countable. Every individual multiset has finite support. This permits state families such as $\{\mathrm{Cu(s)} : \theta : \theta \in \mathbb{N}_0\}$ without contradicting the finite-support requirement.

2.1. Classical structure, hyperstructure, and n-superhyperstructure

Definition 1 (Atomic and multiset state)**.** Let S be a nonempty set of atomic states. Its free commutative multiset monoid is

$$\mathcal{M}(S) = \{x : S \to \mathbb{N}_0 : \mathrm{supp}(x) \text{ is finite}\},$$

with pointwise addition. The basis multiset associated with $s \in S$ is denoted $[s]$. Thus $2[\mathrm{H_2O}]$ records two water molecules, while an ordinary set would lose the coefficient 2.

Definition 2 (Powerset)**.** For a set X, let $\mathcal{P}(X) = \{A : A \subseteq X\}$ and $\mathcal{P}_*(X) = \mathcal{P}(X) \setminus \{\varnothing\}$.

Definition 3 (Iterated nonempty powerset)**.** Define

$$\mathcal{P}_*^0(X) = X, \qquad \mathcal{P}_*^{k+1}(X) = \mathcal{P}_*\left(\mathcal{P}_*^k(X)\right), \quad k \geq 0.$$

The empty set is therefore excluded at every level. When empty outcomes are required, the separate notation $\mathcal{P}^0(X) = X$ and $\mathcal{P}^{k+1}(X) = \mathcal{P}(\mathcal{P}^k(X))$ is used.

Example 1 (A third powerset in emergency planning)**.** For $S = \{\mathrm{AmbA}, \mathrm{AmbB}, \mathrm{Fire}\}$, an element of $\mathcal{P}_*(S)$ is a nonempty deployment, an element of $\mathcal{P}_*^2(S)$ is a nonempty family of deployments, and an element of $\mathcal{P}_*^3(S)$ is a nonempty catalogue of such families. The levels are not identified with one another.

Definition 4 (Classical structure)**.** A classical r-ary operation on a nonempty set H is a total map $f : H^r \to H$. A partial classical operation has a declared domain $D \subseteq H^r$.

Definition 5 (Hyperoperation)**.** An r-ary hyperoperation on H is a map

$$h : D \longrightarrow \mathcal{P}_*(H), \qquad D \subseteq H^r.$$

Its values are nonempty sets of alternative outputs. If infeasible inputs must be represented explicitly, one may instead use a total map $H^r \to \mathcal{P}(H)$, with the empty set denoting infeasibility. The two conventions must not be mixed.

Definition 6 (Hyperstructure)**.** A hyperstructure is a tuple $(H, \Sigma, \{h_\sigma\}_{\sigma\in\Sigma})$, where Σ is a signature, $\mathrm{ar}(\sigma) \geq 1$, and each

$$h_\sigma : D_\sigma \subseteq H^{\mathrm{ar}(\sigma)} \longrightarrow \mathcal{P}_*(H),$$

is a hyperoperation. No associativity, reproduction, or hypergroup axiom is assumed unless stated separately.

Example 2 (ABO inheritance as a hyperoperation)**.** Let $H = \{A, B, AB, O\}$. If unobserved parental genotypes are treated as latent alternatives, the phenotype-level map sends a parental phenotype pair to the set of possible child phenotypes. For example,

$$A \star B = \{A, B, AB, O\}, \quad AB \star O = \{A, B\}, \quad O \star O = \{O\}.$$

This is a hyperoperation on H, not an ordinary operation on $\mathcal{P}(H)$.

Definition 7 ((m,n)-superhyperoperation)**.** Let H be nonempty, let $m \geq 0$, $n \geq 1$, and let $r \geq 1$. An (m,n)-superhyperoperation of arity r is a partial map

$$F^{(m,n)} : D^{(m)} \subseteq \left(\mathcal{P}^m_*(H)\right)^r \longrightarrow \mathcal{P}^n_*(H).$$

The symbols m, n, r have only these meanings throughout the paper.

Definition 8 (n-superhyperstructure)**.** An n-superhyperstructure is the special case $m = n$ of Definition 7. Its carrier is $\mathcal{P}^n_*(H)$, and each operation has a declared subset of $(\mathcal{P}^n_*(H))^r$ as its feasibility domain.

Definition 9 (Constrained superhyperstructure)**.** Let $H = \mathcal{M}(S)$. A constrained (m,n)-superhyperstructure consists of

$$\mathfrak{H}^{(m,n)} = \left(H, \Sigma, \{F^{(m,n)}_\sigma, D^{(m)}_\sigma, \mathrm{Feas}^{(m,n)}_\sigma\}_{\sigma\in\Sigma}, \nu, \Phi, \{C_\sigma\}\right),$$

where

$$F^{(m,n)}_\sigma, \mathrm{Feas}^{(m,n)}_\sigma : D^{(m)}_\sigma \longrightarrow \mathcal{P}^n_*(H), \qquad F^{(m,n)}_\sigma(\mathbf{X}) \subseteq \mathrm{Feas}^{(m,n)}_\sigma(\mathbf{X}),$$

for $n \geq 1$. Here $\nu : H \to \mathbb{Z}^d$ is additive, $\Phi : H \to \mathbb{R}$ is a declared score or potential, and $C_\sigma \subseteq \mathbb{R}^d$ is a closed convex cone. The cone is defined in the vector space $\mathbb{R}^d$, not in an unspecified monoid.

Example 3 (Playlist curation as a $(1,2)$-operation)**.** Let H be a finite set of tracks. An input $A \in \mathcal{P}_*(H)$ is a candidate pool. Define $F^{(1,2)}(A)$ to be the nonempty family of playlists $P \subseteq A$ satisfying declared duration, artist, and tempo constraints. Then $F^{(1,2)}(A) \in \mathcal{P}^2_*(H)$. The example illustrates levels only; it is not used as chemical evidence.

2.2. Chemical Hyperstructure

Definition 10 (Chemical hyperstructure)**.** Let S_{chem} be a set of chemical species and $H_{\mathrm{chem}} = \mathcal{M}(S_{\mathrm{chem}})$. For context θ (temperature, activities, pressure, solvent, and electrode convention), let $\mathrm{Cand}_\sigma(\theta; \mathbf{x}) \subseteq H_{\mathrm{chem}}$ be the candidate product multisets for input $\mathbf{x} \in D_\sigma(\theta)$. Let $\nu : H_{\mathrm{chem}} \to \mathbb{Z}^d$ record elemental and charge balances. A chemical hyperoperation is

$$h_{\sigma,\theta}(\mathbf{x}) = \{y \in \mathrm{Cand}_\sigma(\theta; \mathbf{x}) : \nu(y) - \textstyle\sum_i \nu(x_i) \in C_\sigma,\ \Delta_r G_\theta(\mathbf{x} \to y) \leq \delta_\sigma\}.$$

The candidate set and all conventions used to calculate $\Delta_r G_\theta$ are part of the definition. For an electrochemical cell,

$$E^\circ_{\mathrm{cell}} = E^\circ_{\mathrm{cathode}} - E^\circ_{\mathrm{anode}}, \qquad \Delta_r G^\circ = -nFE^\circ_{\mathrm{cell}},$$

when both tabulated electrode values are reduction potentials [9,10]. Potentials are attached to specified redox couples, not to isolated product species.

Example 4 (Daniell cell)**.** Let

$$S_{\text{chem}} = \{\text{Zn}, \text{Zn}^{2+}, \text{Cu}, \text{Cu}^{2+}\},$$

and use the balanced channel

$$\text{Zn} + \text{Cu}^{2+} \longrightarrow \text{Zn}^{2+} + \text{Cu}.$$

At 298.15 K, representative standard reduction potentials are $E^{\circ}(\text{Cu}^{2+}/\text{Cu}) = +0.340\,\text{V}$ and $E^{\circ}(\text{Zn}^{2+}/\text{Zn}) = -0.763\,\text{V}$ [10]. Therefore

$$E^{\circ}_{\text{cell}} = 0.340 - (-0.763) = 1.103\,\text{V} > 0.$$

The element-charge residual is exactly zero. If this is the only candidate channel, the hyperoperation returns the singleton set containing the product multiset $[\text{Zn}^{2+}] + [\text{Cu}]$.

2.3. Chemical Superhyperstructure

Definition 11 (Chemical superhyperstructure of order (m, n))**.** For $H_{\text{chem}} = \mathcal{M}(S_{\text{chem}})$, the chemical (m, n)-superhyperoperation

$$F^{(m,n)}_{\sigma,\theta} : D^{(m)}_{\sigma}(\theta) \subseteq \left(\mathcal{P}^{m}_{*}(H_{\text{chem}})\right)^{\text{ar}(\sigma)} \longrightarrow \mathcal{P}^{n}_{*}(H_{\text{chem}}),$$

collects nonempty families of admissible product multisets or pathway families. Every elementary edge in every represented path must satisfy Definition 10. A redox selector compares complete, balanced channels under one potential convention; no potential is evaluated on a bare subset.

Example 5 (An order-$(1, 2)$ redox family)**.** Let $X = \{[\text{Zn}] + [\text{Cu}^{2+}]\} \in \mathcal{P}_{*}(H_{\text{chem}})$. The one-channel family

$$\left\{\left\{[\text{Zn}^{2+}] + [\text{Cu}]\right\}\right\} \in \mathcal{P}^{2}_{*}(H_{\text{chem}}),$$

is a valid output. The inner multiset records joint products; the next level records an alternative family. This corrects the ambiguity between co-products and alternative channels.

Proposition 1 (Pathwise preservation of additive balance)**.** *Suppose each elementary channel $x \to y$ satisfies $\nu(y) - \nu(x) \in C$, where $C \subseteq \mathbb{R}^{d}$ is a cone closed under addition. Then every finite path $x_0 \to x_1 \to \cdots \to x_L$ satisfies $\nu(x_L) - \nu(x_0) \in C$.*

Proof. By telescoping and additivity,

$$\nu(x_L) - \nu(x_0) = \sum_{j=1}^{L} \big(\nu(x_j) - \nu(x_{j-1})\big).$$

Every summand belongs to C, and closure of C under addition gives the claim. □

Corollary 1 (Exact conservation)**.** *If $C = \{0\}$, exact balance at every elementary edge implies exact balance along every represented finite pathway.*

Proposition 2 (Reduction)**.** *For $m = 0$ and $n = 1$, Definition 7 has signature $D \subseteq H^{r} \to \mathcal{P}_{*}(H)$, exactly the signature of the hyperoperation in Definition 5. Thus no identification or flattening map is required.*

3. Main result

The main result is the common construction in Definition 9, together with the preservation and reduction statements above. Each specialization below declares its atomic state set, multiset carrier, feasibility data, balance valuation, and selector. The reported checks were performed with exact integer stoichiometric vectors

and double-precision evaluation only for the displayed physical constants. For a channel $x \to y$, the balance residual is

$$\mathrm{Res}_\nu(x \to y) = \nu(y) - \nu(x), \qquad \| \mathrm{Res}_\nu \|_\infty = \max_j | \mathrm{Res}_{\nu,j} |.$$

Zero residual denotes exact balance in all declared components.

For a finite atomic set $S = \{s_1, \ldots, s_q\}$, a multiset is stored as a coefficient vector $x \in \mathbb{N}_0^q$. If the j-th column of $N \in \mathbb{Z}^{d \times q}$ is the balance vector of s_j, then $\nu(x) = Nx$. An elementary channel is represented by nonnegative reactant and product vectors x^-, x^+, and its exact residual is

$$\mathrm{Res}_\nu = N(x^+ - x^-).$$

This matrix calculation is the reproducibility protocol used for the entries in Table 2. It prevents visual inspection of a displayed equation from being mistaken for a balance proof. Reservoir terms, including e^-, $h\nu$, H^+, solvent, and surface-site tokens, must either be columns of N or be recorded in a separate declared residual vector.

Table 2. Compact overview: Hyperoperations return sets of admissible outcomes; SuperHyper (m, n) lifts inputs to $\mathcal{P}_*^m(S)$ and outputs to $\mathcal{P}_*^n(S)$, collecting families of multi-step outcomes under domain-specific constraints.

Domain	Checked channel or quantity	Balance result	Independent selector/check
Biochemical	$S^{(\alpha)} + \mathrm{ATP} + K \to S^{(\alpha \cup \{i\})} + \mathrm{ADP} + K$	phosphate and catalyst residual 0	site $i \notin \alpha$
Geochemical	$Mg_2SiO_4 + 4H^+ \to 2Mg^{2+} + H_4SiO_4$	$\| \mathrm{Res}_\nu \|_\infty = 0$	saturation/$\Delta_r G$ requires environment data
Photochemical	365 nm incident photon	not a stoichiometric reaction	$E_\gamma = 3.3968\,\mathrm{eV}$
Electrochemical	$Zn + Cu^{2+} \to Zn^{2+} + Cu$	$\| \mathrm{Res}_\nu \|_\infty = 0$	$E^\circ_{\mathrm{cell}} = 1.103\,\mathrm{V}$
Electrochemical	$O_2 + 4H^+ + 4e^- \to 2H_2O$	$\| \mathrm{Res}_\nu \|_\infty = 0$	$E^\circ \simeq 1.229\,\mathrm{V}$
Radiochemical	principal ^{212}Bi branches	$\| \mathrm{Res}_{(B,Q,L)} \|_\infty = 0$	$64.06 + 35.94 = 100.00\%$
Neurochemical	DA + D1R → DA:D1R	token residual 0	specificity predicate required
Medicinal-chemical	D + T → D:T	moiety residual 0	fixed normalized score required

The computational construction of a lifted output follows four deterministic steps. First, enumerate or generate the candidate elementary channels applicable to the input multisets. Second, remove candidates whose matrix residual, energetic inequality, or domain-specific predicate fails. Third, compose the remaining channels up to a declared maximum path length L, retaining ordered edge records. Fourth, group the resulting paths at the requested powerset level without flattening product multisets. Ties are retained as distinct alternatives. These steps make the examples reproducible once the candidate generator and numerical parameters are supplied.

Proposition 3 (Finite computability and powerset growth)**.** *If H is finite with $|H| = q$, then*

$$a_0 = q, \qquad a_{k+1} = 2^{a_k} - 1,$$

gives $|\mathcal{P}_*^k(H)| = a_k$. A bounded-length lift is therefore computable by finite enumeration, but unrestricted materialization becomes impractical after very few levels.

Proof. The number of nonempty subsets of a set with a_k elements is $2^{a_k} - 1$. Induction on k gives the formula. Finiteness proves enumerability, while the recurrence shows the tower-like growth. □

Accordingly, the practical representation is sparse: the implementation stores only reachable multisets and reachable pathway families, never the full iterated powerset. This clarifies what the hierarchy adds beyond a reaction graph. The graph or Petri-net layer stores elementary edges and stoichiometry; the superhyperstructure layer stores nonempty alternative families of such paths at explicitly typed levels. The latter is useful only when a scientific question genuinely concerns families of scenarios, policies, or pathway ensembles.

Numerical reporting follows a fixed precision rule. Exact integer residuals are reported as zero without tolerance. Values derived from evaluated constants are calculated at greater precision and rounded only in the displayed result. Thus $0.340 - (-0.763) = 1.103\,\mathrm{V}$, the exact SI constants give $3.396827354\ldots$ eV at 365 nm,

and the evaluated ^{212}Bi principal-branch percentages give $64.06 + 35.94 = 100.00$. These are verification calculations rather than fitted simulation outputs.

3.1. BioChemical HyperStructure

Definition 12 (Biochemical hyperstructure)**.** Let S_{bch} contain biochemical species and declared complex states, and let $H_{\mathrm{bch}} = \mathcal{M}(S_{\mathrm{bch}})$. For each interaction $\sigma \in \Sigma_{\mathrm{bch}}$, specify a domain $D_\sigma(\theta)$, candidate product multisets, an additive balance map ν, an energetic change $\Delta_r G_\theta$, and a mechanistic predicate Sel_σ. Define

$$h_{\sigma,\theta}(\mathbf{x}) = \left\{ y \in \mathrm{Cand}_\sigma(\theta;\mathbf{x}) : \begin{array}{l} \nu(y) - \sum_i \nu(x_i) \in C_\sigma, \\ \Delta_r G_\theta(\mathbf{x} \to y) \le \delta_\sigma, \\ \mathrm{Sel}_\sigma(\mathbf{x} \to y;\theta) \end{array} \right\}.$$

Enzymes are represented on both sides of a catalytic channel; their reproduction is therefore checked by multiset coefficients, not by asking whether a catalyst is itself an alternative output.

Example 6 (Two-site protein phosphorylation)**.** Let $S^{(\alpha)}$ denote a substrate whose modified sites are $\alpha \subseteq \{1,2\}$, and let K be a kinase. For $i \notin \alpha$, use the coarse-grained channel

$$[S^{(\alpha)}] + [\mathrm{ATP}] + [K] \longrightarrow [S^{(\alpha \cup \{i\})}] + [\mathrm{ADP}] + [K].$$

With $\nu_P(S^{(\alpha)}) = |\alpha|$, $\nu_P(\mathrm{ATP}) = 1$, $\nu_P(\mathrm{ADP}) = 0$, and $\nu_K(K) = 1$, both the transferable-phosphate and catalyst-token residuals are zero. If two sites are initially available, the hyperoperation returns two alternative product multisets, one for each i; it does not merge the alternatives into one product set.

3.2. BioChemical SuperHyperStructure

Definition 13 (Biochemical superhyperstructure of order (m,n))**.** The biochemical lift

$$F^{(m,n)}_{\sigma,\theta} : D^{(m)}_\sigma(\theta) \longrightarrow \mathcal{P}^n_*(H_{\mathrm{bch}}),$$

collects families of multiset states reachable through declared biochemical channels. For every represented elementary edge, the balance, energetic, localization, and enzyme-availability predicates of Definition 12 must hold. The feasible-family map $\mathrm{Feas}^{(m,n)}_{\sigma,\theta}$ has the same codomain $\mathcal{P}^n_*(H_{\mathrm{bch}})$, so the inclusion $F^{(m,n)}_{\sigma,\theta}(\mathbf{X}) \subseteq \mathrm{Feas}^{(m,n)}_{\sigma,\theta}(\mathbf{X})$ is well typed.

Example 7 (Two-step phosphorylation–isomerization family)**.** Let $X \in \mathcal{P}_*(H_{\mathrm{bch}})$ contain a substrate, ATP, and kinase. For each phosphorylation alternative, apply a declared unary isomerization channel. The resulting object is a nonempty set of one-step and two-step pathway families in $\mathcal{P}^2_*(H_{\mathrm{bch}})$. Exact token balance follows edge by edge from Proposition 1; no direct comparison of one final atom with the whole initial mixture is used.

3.3. Geochemical HyperStructure

Definition 14 (Geochemical hyperstructure)**.** Let $H_{\mathrm{geo}} = \mathcal{M}(S_{\mathrm{geo}})$, where S_{geo} contains minerals, aqueous species, gases, and explicitly declared reservoir tokens. At environment $e = (T, P, \mathrm{pH}, \mathrm{activities}, f_{\mathrm{O}_2})$, a geochemical hyperoperation returns balanced product multisets satisfying phase, saturation, and $\Delta_r G_e$ predicates. The valuation records elemental counts and electric charge; exchange with an external reservoir must appear either as explicit reactant tokens or as a declared nonzero residual cone.

Example 8 (Balanced forsterite dissolution)**.** At acidic conditions, the channel

$$\mathrm{Mg_2SiO_4(s)} + 4\mathrm{H^+(aq)} \longrightarrow 2\mathrm{Mg^{2+}(aq)} + \mathrm{H_4SiO_4(aq)},$$

has zero residual for $(\mathrm{Mg}, \mathrm{Si}, \mathrm{O}, \mathrm{H}, q)$:

$$(2,1,4,4,+4)_{\mathrm{left}} = (2,1,4,4,+4)_{\mathrm{right}}.$$

Multiplicity is essential: replacing $2[\mathrm{Mg}^{2+}]$ by an ordinary set would make the displayed balance unrecoverable. Thermodynamic or saturation selection requires environment-specific activity data and is not asserted without those data [11].

3.4. Geochemical SuperHyperStructure

Definition 15 (Geochemical superhyperstructure of order (m, n))**.** The geochemical lift maps scenario families in $\mathcal{P}_*^m(H_{\mathrm{geo}})$ to nonempty pathway families in $\mathcal{P}_*^n(H_{\mathrm{geo}})$. Each dissolution, hydrolysis, redox, or precipitation edge must be separately balanced. Environment-dependent predicates are held fixed along one path unless a transition explicitly changes the environment.

Example 9 (Weathering pathway family)**.** A two-step family may combine the balanced forsterite dissolution channel above with a separately balanced carbonate-precipitation channel such as

$$\mathrm{Mg}^{2+} + \mathrm{HCO}_3^- \longrightarrow \mathrm{MgCO_3(s)} + \mathrm{H}^+.$$

The superhyperoperation retains the two edges and their co-products as multisets. Whether the precipitation is feasible is determined by a declared saturation index, not by the powerset construction itself.

3.5. Photochemical HyperStructure

Definition 16 (Photochemical hyperstructure)**.** Let $H_{\mathrm{pho}} = \mathcal{M}(S_{\mathrm{pho}})$, where an atomic state specifies the molecular identity and its electronic, vibrational, and spin labels. Let ℓ specify wavelength, spectral width, polarization, intensity, solvent, and temperature. Each elementary photoprocess has a process label $\rho \in \{\mathrm{abs}, \mathrm{em}, \mathrm{IC}, \mathrm{ISC}, \mathrm{react}\}$ and its own reservoir term $b_\rho(\ell)$. In particular,

$$b_{\mathrm{abs}}(\ell) = [h\nu], \qquad b_{\mathrm{IC}}(\ell) = b_{\mathrm{ISC}}(\ell) = 0.$$

The hyperoperation returns product multisets satisfying the relevant energy window, spin, angular-momentum, and mechanistic predicates. A photon is therefore added only to a photon-absorbing edge, not to every edge in a cascade.

Example 10 (Azobenzene excitation at 365 nm)**.** For the absorption channel

$$[\mathrm{Az\text{-}trans} : S_0] + [h\nu] \longrightarrow [\mathrm{Az\text{-}trans}^* : S_1],$$

the incident photon energy is calculated from exact SI constants:

$$E_\gamma = \frac{hc}{\lambda} = \frac{(6.62607015 \times 10^{-34}\,\mathrm{J\,s})\,(299792458\,\mathrm{m\,s^{-1}})}{365 \times 10^{-9}\,\mathrm{m}} = 3.396827\ldots\ \mathrm{eV}.$$

The reported value is 3.3968 eV after rounding. It is an irradiation energy, not an assertion that a specific molecular transition is exactly resonant; that decision requires a measured or calculated absorption band [12, 13].

3.6. Photochemical SuperHyperStructure

Definition 17 (Photochemical superhyperstructure of order (m, n))**.** The photochemical lift collects nonempty families of elementary, type-labeled photochemical paths. For every edge $x_{j-1} \xrightarrow{\rho_j} x_j$, the balance test uses only b_{ρ_j}. Consequently, one absorption followed by internal conversion consumes one photon in total, rather than one photon per path edge. Multimolecular edges retain their full multiset inputs.

Example 11 (Sensitized singlet-oxygen pathway)**.** A valid path is represented by separate edges:

$$\begin{aligned}
&[\text{Sens} : S_0] + [h\nu] \to [\text{Sens} : S_1],\\
&[\text{Sens} : S_1] \to [\text{Sens} : T_1],\\
&[\text{Sens} : T_1] + [\text{O}_2(^3\Sigma_g^-)] \to [\text{Sens} : S_0] + [\text{O}_2(^1\Delta_g)],\\
&[\text{O}_2(^1\Delta_g)] + [\text{Sub}] \to [\text{Sub-ox}].
\end{aligned}$$

The third and fourth lines are binary channels; they are not generated from a single atomic input. A $(1, 2)$ operation may collect the resulting pathway alternatives only when the input scenario multiset contains the required sensitizer, oxygen, and substrate tokens.

3.7. Electrochemical HyperStructure

Definition 18 (Electrochemical hyperstructure)**.** Let $H_{\text{ele}} = \mathcal{M}(S_{\text{ele}})$ and include the electron reservoir token e^- whenever charge is checked stoichiometrically. At environment ϵ and applied potential U, define the grand potential

$$\Psi_{\epsilon,U}(x) = G_\epsilon(x) + \mu_e(U)n_e(x), \qquad \mu_e(U) = -FU,$$

under a stated sign convention. An elementary electrochemical hyperoperation returns balanced product multisets that satisfy

$$\nu(y) = \nu(x), \qquad \Psi_{\epsilon,U}(y) - \Psi_{\epsilon,U}(x) \le \delta_\sigma,$$

and any declared mass-transport, site-availability, Nernst, or kinetic predicate. Electron transfer is not declared charge balanced unless the electron-reservoir coefficient is included in ν.

Example 12 (Copper deposition and hydrogen evolution)**.** The two competing cathodic processes require different complete input multisets:

$$\begin{aligned}
[\text{Cu}^{2+}] + 2[e^-] + [*] &\longrightarrow [\text{Cu}{-}*],\\
2[\text{H}^+] + 2[e^-] + 2[*] &\longrightarrow [\text{H}_2] + 2[*].
\end{aligned}$$

Here $*$ denotes a surface-site token. Both equations have zero elemental and electric-charge residual. They may compete at one electrode potential when both solution reactants are available, but metal deposition is not an outcome of the input $(\text{H}^+, \text{surface})$ alone [14].

3.8. Electrochemical SuperHyperStructure

Definition 19 (Electrochemical superhyperstructure of order (m, n))**.** For fixed (ϵ, U), define

$$F^{(m,n)}_{\sigma,\epsilon,U} : D^{(m)}_\sigma(\epsilon, U) \subseteq \left(\mathcal{P}^m_*(H_{\text{ele}})\right)^{\text{ar}(\sigma)} \longrightarrow \mathcal{P}^n_*(H_{\text{ele}}).$$

The feasible-family map has the same codomain and enforces site capacity, mass transport, balanced proton-coupled electron transfer, potential-dependent energetics, and declared kinetic filters. This definition replaces the duplicated ordinary electrochemical definition that would otherwise leave the lifted symbols undefined.

Example 13 (Four- and two-electron oxygen reduction)**.** In acidic solution, the net channels are

$$\begin{aligned}
\text{O}_2 + 4\text{H}^+ + 4e^- &\longrightarrow 2\text{H}_2O, \quad E^\circ \simeq 1.229\,\text{V},\\
\text{O}_2 + 2\text{H}^+ + 2e^- &\longrightarrow \text{H}_2O_2, \quad E^\circ \simeq 0.695\,\text{V}.
\end{aligned}$$

Both equations have zero (O, H, q) residual. The product $2[\text{H}_2O]$ remains distinct from $[\text{H}_2O]$, and the two pathways remain distinct alternatives in $\mathcal{P}^2_*(H_{\text{ele}})$. The standard potentials describe thermodynamic reference states; they do not predict rates, selectivity, or overpotential without a kinetic model [15].

3.9. Radiochemical HyperStructure

Definition 20 (Radiochemical hyperstructure)**.** Let $H_{\mathrm{rad}} = \mathcal{M}(S_{\mathrm{rad}})$, with atomic states for nuclides and emitted particles. Use the additive valuation

$$\nu = (B, Q, L),$$

where B is baryon number, Q is electric charge in units of e, and L is lepton number when leptons occur. Proton number Z is a nuclide label, not a conserved component in beta transformation. A radiochemical hyperoperation returns nonempty sets of channels satisfying these additive invariants, a positive decay Q-value or other declared energetic condition, and the applicable angular-momentum and parity rules.

Example 14 (Competing ^{212}Bi branches)**.** The two principal evaluated branches are

$$\begin{aligned} {}^{212}_{83}\mathrm{Bi} &\longrightarrow {}^{212}_{84}\mathrm{Po} + e^- + \bar{\nu}_e, \quad b_{\beta^-} = 64.06\%, \quad Q_{\beta^-} = 2.2521\,\mathrm{MeV}, \\ {}^{212}_{83}\mathrm{Bi} &\longrightarrow {}^{208}_{81}\mathrm{Tl} + {}^{4}_{2}\mathrm{He}, \qquad\quad b_{\alpha} = 35.94\%, \qquad Q_{\alpha} = 6.20726\,\mathrm{MeV}. \end{aligned}$$

The evaluated branching fractions sum to 100.00% at the reported precision [16]. For the beta channel,

$$(B, Q, L)_{\mathrm{left}} = (212, 83, 0) = (212, 84, 0) + (0, -1, 1) + (0, 0, -1),$$

and the alpha channel similarly conserves B and Q. Thus both channels have zero residual under the corrected valuation.

3.10. Radiochemical SuperHyperStructure

Definition 21 (Radiochemical superhyperstructure of order (m, n))**.** The radiochemical lift collects nonempty families of balanced nuclear channels and finite decay paths:

$$F^{(m,n)}_{\sigma,\eta} : D^{(m)}_{\sigma}(\eta) \longrightarrow \mathcal{P}^{n}_{*}(H_{\mathrm{rad}}).$$

Every represented channel retains all emitted-particle coefficients. If an output is required to contain exactly two generations, its defining predicate requires a two-edge path and a two-element ordered path record; it is not defined as an arbitrary subset that may be empty or omit an edge.

Example 15 (Two-generation ^{212}Bi families)**.** Two principal path alternatives are

$$^{212}\mathrm{Bi} \xrightarrow{\alpha} {}^{208}\mathrm{Tl} \xrightarrow{\beta^-} {}^{208}\mathrm{Pb}, \qquad {}^{212}\mathrm{Bi} \xrightarrow{\beta^-} {}^{212}\mathrm{Po} \xrightarrow{\alpha} {}^{208}\mathrm{Pb}.$$

Each edge is stored as a complete product multiset, while the ordered pair of edges records one two-generation path. Conservation for the full path follows from Proposition 1. Branching probabilities may be attached as weights, but weights are additional data and are not generated by the powerset operator.

3.11. Neurochemical HyperStructure

Definition 22 (Neurochemical hyperstructure)**.** Let $H_{\mathrm{neu}} = \mathcal{M}(S_{\mathrm{neu}})$, where states include transmitters, receptors in declared conformations, transporters, enzymes, and complexes. Each process has a complete microstate multiset as input. A neurochemical hyperoperation returns product multisets satisfying molecule-token balance, receptor or transporter specificity, compartment availability, and a separately declared kinetic or probabilistic rule. If approximate pool balance is needed, define a metric d on the valuation space and impose $d(\nu(y), \nu(x)) \leq \Delta_{\sigma}$; a norm is not assumed on a bare monoid.

Example 16 (Dopamine binding and reuptake channels)**.** With explicit tokens, representative channels include

$$[\mathrm{DA}] + [\mathrm{D1R}_{\mathrm{inact}}] \longrightarrow [\mathrm{DA{:}D1R}^*], \qquad [\mathrm{DA}] + [\mathrm{DAT}] \longrightarrow [\mathrm{DAT{:}DA}].$$

For a valuation that counts dopamine, receptor, and transporter moieties, both channels have zero residual. A synaptic "baseline" is represented as a multiset of all available tokens, not as one undefined atomic state. Affinities, concentrations, and rate constants must be supplied before the model makes quantitative occupancy or time-course predictions [17].

3.12. Neurochemical SuperHyperStructure

Definition 23 (Neurochemical superhyperstructure of order (m,n))**.** The neurochemical lift maps scenario families of complete synaptic microstates to nonempty families of receptor-binding, transport, degradation, and recycling paths. Each path edge has its own arity and specificity predicate. Resource drift is evaluated between complete parent and child multisets using the declared metric; it is not simultaneously asserted to be nonzero and exactly zero.

Example 17 (Binding–reuptake pathway families)**.** For a scenario containing dopamine, receptor, and transporter tokens, one family may contain a binding edge followed by receptor release, while another contains transporter binding followed by intracellular transport. The alternatives are stored separately, and token balance is checked per edge. This construction represents possible pathway families but does not replace stochastic kinetic modeling.

3.13. Medichemical HyperStructure

Definition 24 (Medicinal-chemical hyperstructure)**.** Let $H_{\mathrm{med}} = \mathcal{M}(S_{\mathrm{med}})$, with atoms for ligands, targets, off-targets, metabolites, and declared complexes. For context θ, specify Cand_σ, a balance map ν, a mechanistic predicate, and a dimensionless score

$$\Phi_\theta(y) = \sum_{j=1}^{k} w_j z_j(y), \qquad w_j \geq 0, \quad \sum_j w_j = 1,$$

where each z_j is explicitly normalized and the direction of preference is stated. The hyperoperation is

$$h_{\sigma,\theta}(\mathbf{x}) = \operatorname*{arg\,min}_{y \in \mathrm{Feas}_\sigma(\theta;\mathbf{x})} \Phi_\theta(y).$$

The weights, normalizations, candidate generator, and tie convention are part of the model. Free energies, toxicity measurements, and ADMET descriptors are not added without normalization because they have different units and uncertainties [18,19].

3.14. Medichemical SuperHyperStructure

Definition 25 (Medicinal-chemical superhyperstructure of order (m,n))**.** For $n \geq 1$, let

$$\mathrm{Cand}_\sigma^{(m,n)}, \mathrm{Feas}_\sigma^{(m,n)} : D_\sigma^{(m)}(\theta) \longrightarrow \mathcal{P}_*^n(H_{\mathrm{med}}).$$

Define

$$F_{\sigma,\theta}^{(m,n)}(\mathbf{X}) = \operatorname*{arg\,min}_{Y \in \mathrm{Feas}_\sigma^{(m,n)}(\mathbf{X})} \mathrm{Agg}_\theta(Y),$$

where Agg_θ is fixed in advance and its argmin is interpreted as the nonempty set of minimizing alternatives at the appropriate level. At $(m,n) = (0,1)$, choosing $\mathrm{Agg}_\theta([y]) = \Phi_\theta(y)$ gives Definition 24 exactly. No extra powerset or informal identification is introduced.

4. Conclusion

This paper has provided a common, type-consistent framework for hierarchical set-valued chemical models. The essential correction is to place reaction multisets, rather than bare species, in the carrier of the hyperoperation. This separates joint co-products from alternative channels and preserves stoichiometric multiplicity. Iterated nonempty powersets are then defined recursively, with distinct symbols for input level,

output level, and arity. The $(0,1)$ reduction is exact, and additive balance is preserved along every finite admissible path.

The domain examples demonstrate what the construction can and cannot establish. Balanced equations, evaluated constants, and explicit residuals support internal mathematical consistency. The framework alone does not generate thermodynamic data, kinetic parameters, branching probabilities, binding affinities, or biological outcomes; these must be supplied from experiment or validated computation. Future work should implement the structures in machine-readable form, analyze the combinatorial growth of iterated powersets, compare reachability with Petri-net and rule-based models, and test predictive performance on domain-specific datasets.

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