An Introduction and Reexamination of Molecular Hypergraph and Molecular n-SuperHypergraph

Abstract

A *molecular graph* is a labeled graph in which atoms are represented by vertices and covalent bonds by edges, with each edge labeled according to the bond type [46]. A *hypergraph* generalizes the concept of a traditional graph by allowing edges—called *hyperedges*—to connect more than two vertices simultaneously [13]. A *superhypergraph* further extends this idea by incorporating recursively defined powerset layers, enabling hierarchical and self-referential relationships among hyperedges [100].

This paper investigates the formalization, illustrative examples, and structural properties of *molecular hypergraphs* and *molecular superhypergraphs* (cf. [28]). These constructs, grounded in the theoretical foundations of hypergraphs and superhypergraphs, provide enriched frameworks for representing molecular systems and facilitate deeper exploration of hierarchical chemical connectivity and molecular structure.

Keywords: Superhypergraph, Hypergraph, Molecular Graph, Molecular n-SuperHypergraph, Molecular HyperGraph

1 Introduction

1.1 Graph, HyperGraph, and SuperHyperGraph

Graph theory is a branch of mathematics that studies the properties of networks, where nodes (called vertices) are connected by links (called edges) [22,23]. Graphs have been extensively studied for applications in various fields such as social science [67,90], graph neural networks (GNNs) [8,37,127], and network analysis [71,73].

Mathematical structures can often be extended into hyperstructures and superhyperstructures by utilizing the power set and n-th iterated powerset constructions (cf. [18,53,101]). These generalized frameworks are particularly well-suited for modeling hierarchical and multi-layered structures across a wide range of conceptual and applied domains. A hypergraph generalizes classical graphs by allowing an edge—called a hyperedge—to connect more than two vertices simultaneously [13,15]. A superhypergraph takes this further by employing recursively nested powerset structures, enabling hierarchical and self-similar relationships among hyperedges themselves [40,99].

The overview of Graph, HyperGraph, and SuperHyperGraph is presented in Table 1.

Concept	Notation	Edge Connectivity	Structural Extension
Graph	$G = (V, E)$	$E \subseteq \{\{u, v\} \mid u, v \in V,\ u \neq v\}$ (binary edges)	Standard graph: edges join exactly two vertices.
HyperGraph	$H = (V, E)$	$E \subseteq \mathcal{P}(V) \setminus \{\emptyset\}$ (hyperedges)	Generalizes edges to connect any nonempty subset of vertices.
SuperHyperGraph	$\mathrm{SHT}^{(n)} = (V, E)$	$V, E \subseteq \mathcal{P}^n(V_0)$ (super-vertices/edges)	Uses n-fold iterated powersets to model hierarchical, nested connectivity among edges.

Table 1: Overview of Graph, HyperGraph, and SuperHyperGraph

1.2 Graph Theory in Chemistry

Chemistry is the scientific study of matter, including its properties, structure, composition, and interactions [27, 89]. Graphs are widely used in the field of chemistry to represent and analyze molecular structures [12,24,68]. Several types of graphs—such as *molecular graphs* [46,58,66,126] and *pharmacophore graphs* [93,119]—have been extensively studied and routinely applied in chemical modeling and analysis.

A molecular graph is a labeled graph in which atoms are represented by vertices and covalent bonds by edges, with each edge labeled according to its bond type. Molecular graphs are often referred to as *chemical graphs*, and the study of chemical graphs has developed into an active area of research [31, 45, 108, 114]. Furthermore, hypergraphs have been introduced as a generalization to capture higher-order interactions in molecules. In particular, *molecular hypergraphs*—defined using hypergraphs—offer a richer and more flexible framework for representing complex chemical connectivity [61, 62].

1.3 Our Contribution

This subsection outlines the contributions of the present paper. This paper investigates the construction and properties of molecular hypergraphs and molecular superhypergraphs, which are extensions of classical graph structures using hypergraph and superhypergraph frameworks (cf. [28]). Through thesee generalizations, we aim to contribute to the advancement of hierarchical modeling in chemistry, providing new perspectives on complex molecular structures. As this paper is purely theoretical, we hope that future work will involve various experimental validations and applications based on the proposed models.

The overview of Molecular Graph, Molecular HyperGraph, and Molecular SuperHyperGraph is presented in Table 2.

Concept	**Notation**	**Elements**	**Labeling**	**Key Feature**
Molecular Graph	$G = (V, E, \ell_V, \ell_E)$	V: atoms, $E \subseteq \{\{u, v\}\}$: covalent bonds	ℓ_V: atomic symbols, ℓ_E: bond orders	Standard pairwise connectivity
Molecular HyperGraph	$H = (V_H, E_H, \ell_V^H, \ell_E^H)$	V_H: bonds as nodes, $E_H \subseteq \mathcal{P}(V_H)$: atoms as hyperedges	ℓ_V^H: bond types, ℓ_E^H: atom types	Captures multi-bond incidences to atoms
Molecular n-SuperHyperGraph	$\mathrm{SH}^{(n)} = (V, E, \ell_V, \ell_E)$	$V \subseteq \mathcal{P}^n(V_0)$: nested groupings of bonds/atoms, $E \subseteq \mathcal{P}^n(V_0)$	Inherited labeling at each level	Models hierarchical, multi-level abstractions of molecular structure

Table 2: Overview of Molecular Graph, Molecular HyperGraph, and Molecular SuperHyperGraph

1.4 Structure of This Paper

This section outlines the structure of the present paper. Section 2 provides concise explanations of fundamental concepts, including Classical Structures, Hyperstructures, n-SuperHyperstructures, HyperGraphs, and n-SuperHyperGraphs. Section 3 introduces the concept of Molecular Hypergraphs. Section 4 presents concrete examples and several mathematical properties of Molecular n-SuperHyperGraphs. Section 5 offers concluding remarks and discusses potential directions for future research.

2 Preliminaries and Definitions

This section provides an overview of the fundamental concepts and definitions essential for the discussions in this paper. Throughout this work, all graphs are assumed to be *undirected*, *finite*, and *simple*, unless stated otherwise.

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, and an *n-Superhyperstructure* can be defined using the n-th powerset [102]. Intuitively, the n-th powerset is a repeated application of the powerset operation. Relevant definitions and simple examples are provided below.

Definition 2.1 (Set). [56] A *set* is a well-defined collection of distinct objects, called elements or members.

Definition 2.2 (Subset)**.** [56] Let A and B be sets. We say that A is a *subset* of B, written $A \subseteq B$, if every element of A is also an element of B; that is,

$$A \subseteq B \iff \forall x\,(x \in A \Rightarrow x \in B).$$

Definition 2.3 (Base Set)**.** A *base set* S is the foundational set from which complex structures such as powersets and hyperstructures are derived. It is formally defined as:

$$S = \{x \mid x \text{ is an element within a specified domain}\}.$$

All elements in constructs like $\mathcal{P}(S)$ or $\mathcal{P}_n(S)$ originate from the elements of S.

Definition 2.4 (Powerset)**.** [33] The *powerset* of a set S, denoted $\mathcal{P}(S)$, is the collection of all possible subsets of S, including both the empty set and S itself. Formally, it is expressed as:

$$\mathcal{P}(S) = \{A \mid A \subseteq S\}.$$

Example 2.5 (Pizza Toppings as a Powerset)**.** Suppose a pizzeria offers three optional toppings:

$$S = \{\text{Pepperoni, Mushrooms, Onions}\}.$$

Then the powerset

$$\mathcal{P}(S) = \{\, A \mid A \subseteq S \,\}$$

consists of all eight possible topping combinations:

$$\emptyset, \quad \{\text{Pepperoni}\}, \quad \{\text{Mushrooms}\}, \quad \{\text{Onions}\},$$
$$\{\text{Pepperoni, Mushrooms}\}, \quad \{\text{Pepperoni, Onions}\}, \quad \{\text{Mushrooms, Onions}\}, \quad \{\text{Pepperoni, Mushrooms, Onions}\}.$$

- $\emptyset$: a plain cheese pizza (no toppings).
- $\{\text{Pepperoni}\}, \{\text{Mushrooms}\}, \{\text{Onions}\}$: pizzas with exactly one topping.
- $\{\text{Pepperoni, Mushrooms}\}, \{\text{Pepperoni, Onions}\}, \{\text{Mushrooms, Onions}\}$: pizzas with two toppings.
- $\{\text{Pepperoni, Mushrooms, Onions}\}$: the fully loaded pizza with all three toppings.

Thus the powerset $\mathcal{P}(S)$ succinctly enumerates every possible pizza order, illustrating how the powerset captures all combinations in a real-world customization scenario.

Definition 2.6 (n-th Powerset)**.** (cf. [28, 33, 97, 102])

The n-th powerset of a set H, denoted $P_n(H)$, is defined iteratively, starting with the standard powerset. The recursive construction is given by:

$$P_1(H) = P(H), \quad P_{n+1}(H) = P(P_n(H)), \quad \text{for } n \geq 1.$$

Similarly, the n-th non-empty powerset, denoted $P_n^*(H)$, is defined recursively as:

$$P_1^*(H) = P^*(H), \quad P_{n+1}^*(H) = P^*(P_n^*(H)).$$

Here, $P^*(H)$ represents the powerset of H with the empty set removed.

Example 2.7 (Travel Itinerary Planning via n-th Powersets)**.** Travel Itinerary Planning involves organizing destinations, schedules, accommodations, and activities to efficiently manage time and experiences during a trip (cf. [16, 92, 95]). Suppose you have three cities you might visit on vacation:

$$H = \{\text{Paris, Rome, Berlin}\}.$$

- $P_1(H) = \mathcal{P}(H)$ is the set of all possible *one-week itineraries*, namely

  $$\{\, \emptyset, \{\text{Paris}\}, \{\text{Rome}\}, \{\text{Berlin}\}, \{\text{Paris, Rome}\}, \{\text{Paris, Berlin}\}, \{\text{Rome, Berlin}\}, \{\text{Paris, Rome, Berlin}\}\}.$$

  Each nonempty subset corresponds to the set of cities you plan to visit in a single week.

- $P_2(H) = \mathcal{P}(P_1(H))$ is the collection of all possible *multi-week travel plans*, where each element is a set of one-week itineraries. For example,

$$X = \big\{\{\text{Paris}\},\ \{\text{Rome}, \text{Berlin}\}\big\}$$

could represent a two-week vacation: Week 1 in Paris, Week 2 in Rome and Berlin.

- $P_3(H) = \mathcal{P}(P_2(H))$ then represents *seasonal trip series*, each element being a set of multi-week plans. For instance,

$$Y = \Big\{\{\{\text{Paris}\}, \{\text{Rome}\}\},\ \{\{\text{Berlin}\}, \{\text{Paris}, \text{Berlin}\}\}\Big\}$$

might encode two distinct two-week itineraries you alternate across the year.

Thus the n-th powerset $P_n(H)$ captures progressively higher "meta" levels of travel organization:

$$\underbrace{\text{Cities}}_{H} \to \underbrace{\text{Weekly Itineraries}}_{P_1(H)} \to \underbrace{\text{Multi-Week Plans}}_{P_2(H)} \to \underbrace{\text{Seasonal Series}}_{P_3(H)} \to \dots$$

This illustrates a concrete, real-world use of iterated powersets in hierarchical trip planning.

The Overview of Set, Powerset, and n-th Powerset is presented in Table 3.

Concept	**Notation**	**Definition**	**Key Feature / Example**
Set	S	A well-defined collection of distinct objects, called elements.	e.g. $S = \{a, b, c\}$.
Powerset	$\mathcal{P}(S)$	The collection of all subsets of S, including $\emptyset$ and S itself.	e.g. $\mathcal{P}(\{a, b\}) = \{\emptyset, \{a\}, \{b\}, \{a, b\}\}$.
n-th Powerset	$P_n(S)$	Defined recursively by $P_1(S) = \mathcal{P}(S)$, $P_{n+1}(S) = \mathcal{P}(P_n(S))$.	e.g. $P_2(\{a, b\}) = \mathcal{P}(\mathcal{P}(\{a, b\}))$.

Table 3: Overview of Set, Powerset, and n-th Powerset

Definition 2.8 (Classical Structure)**.** (cf. [97, 102]) 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 2.9 (Hyperoperation)**.** (cf. [112, 113]) 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 2.10 (Hyperstructure)**.** (cf. [33, 102]) A *Hyperstructure* extends the notion of a Classical Structure by operating on the powerset of a base set. Formally, it is defined as:

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

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.

Example 2.11 (Chemical Reaction Hyperstructure)**.** A Chemical Reaction is a process where substances (reactants) are transformed into new substances (products) through the rearrangement of atoms (cf. [3, 21]). Consider the set of chemical species

$$S = \{ \mathrm{H_2},\ \mathrm{O_2},\ \mathrm{H_2O},\ \mathrm{H_2O_2}\},$$

where H_2 is hydrogen gas, O_2 is oxygen gas, H_2O is water, and H_2O_2 is hydrogen peroxide.

Hyperoperation $\circ$: The reaction hyperoperation

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

is defined on pure reagents by:

$$\mathrm{H_2} \circ \mathrm{O_2} = \{\mathrm{H_2O}, \mathrm{H_2O_2}\}, \quad \mathrm{H_2} \circ \mathrm{H_2} = \{\mathrm{H_2}\}, \quad \mathrm{O_2} \circ \mathrm{O_2} = \{\mathrm{O_2}\},$$

and extended symmetrically (so $a \circ b = b \circ a$), with all other combinations yielding the singleton of one reactant when no reaction occurs.

Hyperstructure $\mathcal{H}$: We then form the hyperstructure

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

where the domain is the powerset $\mathcal{P}(S)$ of all subsets of species, and the hyperoperation is extended to mixtures by

$$A \circ B = \bigcup_{a \in A,\ b \in B} (a \circ b), \quad A, B \subseteq S.$$

Concrete computation:

$$\{\mathrm{H_2}\} \circ \{\mathrm{O_2}\} = \{\mathrm{H_2O}, \mathrm{H_2O_2}\}, \quad \{\mathrm{H_2}, \mathrm{O_2}\} \circ \{\mathrm{O_2}\} = (\mathrm{H_2} \circ \mathrm{O_2}) \cup (\mathrm{O_2} \circ \mathrm{O_2}) = \{\mathrm{H_2O}, \mathrm{H_2O_2}, \mathrm{O_2}\}.$$

Thus $\mathcal{H}$ models real-world chemical mixing: combining reagents yields a set of possible products, and mixing mixtures yields the union of all individual reaction outcomes, capturing both single-step and multi-step processes within one algebraic framework.

Definition 2.12 (SuperHyperOperations)**.** (cf. [102]) 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:

$$\mathcal{P}^0(H) = H, \quad \mathcal{P}^{k+1}(H) = \mathcal{P}(\mathcal{P}^k(H)), \quad \text{for } k \geq 0.$$

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 2.13 (n-Superhyperstructure)**.** (cf. [30, 34, 102]) An *n-Superhyperstructure* further generalizes a Hyperstructure by incorporating the n-th powerset of a base set. It is formally described as:

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

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 2.14 (Smartphone Product Bundling as a 2-Superhyperstructure)**.** Smartphone Product Bundling combines a smartphone with accessories or services, offering them together as a single package to increase value. Let the base set of components be

$$S = \{\text{Frame, Screen, Battery, CircuitBoard}\}.$$

First-level collections (modules, in $\mathcal{P}_1(S)$) are:

$$M_1 = \{\text{Frame}, \text{Screen}\}, \quad M_2 = \{\text{Battery}, \text{CircuitBoard}\}, \quad M_3 = \{\text{Screen}, \text{Battery}\}.$$

Second-level collections (product bundles, in $\mathcal{P}_2(S)$) are:

$$P_1 = \{M_1, M_2\}, \quad P_2 = \{M_1, M_3\}, \quad P_3 = \{M_2, M_3\}.$$

Thus $\mathcal{P}_2(S) = \{P_1, P_2, P_3\}$. We define the hyperoperation

$$\circ \; : \; \mathcal{P}_2(S) \times \mathcal{P}_2(S) \longrightarrow \mathcal{P}\big(\mathcal{P}_2(S)\big)$$

by

$$X \circ Y = \big\{ X \cup Y, \; X \cap Y, \; (X \cup Y) \setminus (X \cap Y) \big\}.$$

Concretely, for two product bundles X and Y:

- $X \cup Y$ is the combined bundle containing every module from both X and Y.
- $X \cap Y$ is the common-module bundle shared by X and Y.
- $(X \cup Y) \setminus (X \cap Y)$ is the exclusive-module bundle (modules present in one bundle but not both).

Therefore $\big(\mathcal{P}_2(S), \circ\big)$ is a 2-Superhyperstructure that models all possible ways to merge, intersect, and differentiate smartphone product bundles in a supply-chain or sales context.

The overview of Classical Structure, Hyperstructure, and n-Superhyperstructure is presented in Table 4.

Concept	**Notation**	**Underlying Set**	**Operation**	**Key Feature**
Classical Structure	$(H, \{\#_0\})$	H	$\#_0 : H^m \to H$	Single-valued operations satisfying algebraic axioms
Hyperstructure	$(\mathcal{P}(S), \circ)$	$\mathcal{P}(S)$	$\circ : S \times S \to \mathcal{P}(S)$ extended to $\mathcal{P}(S) \times \mathcal{P}(S)$	Operations yield sets of results (multi-valued)
n-Superhyperstructure	$(\mathcal{P}^n(S), \circ)$	$\mathcal{P}^n(S)$	$\circ : \mathcal{P}^n(S) \times \mathcal{P}^n(S) \to \mathcal{P}^n(S)$	Hierarchical, nested operations via iterated powersets

Table 4: Overview of Classical Structure, Hyperstructure, and n-Superhyperstructure

2.2 SuperHyperGraph

In classical graph theory, a hypergraph extends the idea of a conventional graph by permitting edges—called hyperedges—to join more than two vertices. This broader framework enables the modeling of more intricate relationships between elements, thereby enhancing its utility in various fields [13,26,50,51]. Related concepts to HyperGraphs include Fuzzy HyperGraphs [7,82,94], Directed HyperGraphs [69,70,81], and Neutrosophic HyperGraphs [6,75]. A *SuperHyperGraph* is an advanced extension of the hypergraph concept, integrating recursive powerset structures into the classical model. This concept has been recently introduced and extensively studied in the literature [2,43,80,86].

Definition 2.15 (Graph)**.** [22] A graph is a mathematical structure consisting of a set of vertices and a set of edges, where each edge connects a pair of distinct vertices.

Definition 2.16 (Hypergraph)**.** [13,15] A *hypergraph* $H = (V(H), E(H))$ consists of:

- A nonempty set $V(H)$ of vertices.
- A set $E(H)$ of hyperedges, where each hyperedge is a nonempty subset of $V(H)$, thereby allowing connections among multiple vertices.

Unlike standard graphs, hypergraphs are well-suited to represent higher-order relationships. In this paper, we restrict ourselves to the case where both $V(H)$ and $E(H)$ are finite.

Example 2.17 (Online Retail Transactions as a Hypergraph)**.** Online Retail Transactions involve purchasing goods or services over the internet, typically recorded as customer-item interactions within digital systems (cf. [1,83]). Consider an online store offering four products:

$$P = \{\text{Laptop, Headphones, Smartphone, Charger}\}.$$

We model customer purchase transactions as a hypergraph $H = (V(H), E(H))$ by letting each product be a vertex:

$$V(H) = \{v_1, v_2, v_3, v_4\} = \{\text{Laptop, Headphones, Smartphone, Charger}\},$$

and each transaction as a hyperedge:

$$E(H) = \big\{e_1 = \{\text{Laptop, Headphones}\},\ e_2 = \{\text{Headphones, Smartphone, Charger}\},\ e_3 = \{\text{Laptop, Charger}\}\big\}.$$

Concretely:

- e_1: a customer bought a Laptop and Headphones together.
- e_2: a customer purchased Headphones, a Smartphone, and a Charger in one order.
- e_3: a customer bought a Laptop and a Charger together.

Thus the hypergraph H captures both pairwise and three-item purchase patterns in the store's transaction data.

Definition 2.18 (n-SuperHyperGraph)**.** [35,39,99,100]
Let V_0 be a finite base set of vertices. For each integer $k \geq 0$, define the iterative powerset by

$$\mathcal{P}^0(V_0) = V_0, \quad \mathcal{P}^{k+1}(V_0) = \mathcal{P}(\mathcal{P}^k(V_0)),$$

where $\mathcal{P}(\cdot)$ denotes the usual powerset operation. An *n-SuperHyperGraph* is then a pair

$$\mathrm{SHT}^{(n)} = (V, E),$$

with

$$V \subseteq \mathcal{P}^n(V_0) \quad \text{and} \quad E \subseteq \mathcal{P}^n(V_0).$$

Each element of V is called an *n-supervertex* and each element of E an *n-superedge*.

Example 2.19 (Global Supply Distribution as a 2-SuperHyperGraph)**.** (cf. [79, 96]) A global manufacturer sources raw materials from multiple suppliers and distributes products via local distribution centers and regional hubs. We model this as a 2-SuperHyperGraph.

Base set of suppliers:

$$V_0 = \{ S_1, S_2, S_3, S_4\},$$

where S_i denotes Supplier i.

Local distribution centers (1-supervertices in $\mathcal{P}^1(V_0)$):

$$\mathrm{DC}_1 = \{S_1, S_2\}, \quad \mathrm{DC}_2 = \{S_3, S_4\}, \quad \mathrm{DC}_3 = \{S_2, S_3\}.$$

Each DC_j collects materials from its member suppliers.

Regional hubs (2-supervertices in $\mathcal{P}^2(V_0)$):

$$\mathrm{Hub}_A = \{\mathrm{DC}_1, \mathrm{DC}_2\}, \quad \mathrm{Hub}_B = \{\mathrm{DC}_2, \mathrm{DC}_3\}.$$

Each hub aggregates goods from two local centers.

2-SuperHyperGraph:

$$\mathrm{SHT}^{(2)} = (V, E), \quad V = \{\mathrm{Hub}_A, \mathrm{Hub}_B\}, \quad E = \big\{\{\mathrm{Hub}_A, \mathrm{Hub}_B\}\big\}.$$

The single hyperedge $\{\mathrm{Hub}_A, \mathrm{Hub}_B\}$ represents the national distribution corridor linking the two regions.

Interpretation: This structure captures a three-tier hierarchy:

$$\underbrace{S_i}_{\text{suppliers}} \longrightarrow \underbrace{\mathrm{DC}_j}_{\substack{\text{local}\\ \text{centers}}} \longrightarrow \underbrace{\mathrm{Hub}_k}_{\substack{\text{regional}\\ \text{hubs}}} \longrightarrow \underbrace{\{\mathrm{Hub}_A, \mathrm{Hub}_B\}}_{\text{national corridor}}.$$

Thus $\mathrm{SHT}^{(2)}$ provides a unified hypergraph view of supplier-center-hub relationships in global supply distribution.

Example 2.20 (Corporate Divisional Structure as a 2-SuperHyperGraph)**.** A Corporate Divisional Structure organizes a company into semi-autonomous units based on products, services, markets, or geographical regions (cf. [25, 117]). Let $V_0 = \{\mathrm{Alice}, \mathrm{Bob}, \mathrm{Carol}, \mathrm{Dave}, \mathrm{Eve}\}$ be the set of individual employees in a company. We first form the following committees (1-supervertices in $\mathcal{P}^1(V_0)$):

$$C_1 = \{\mathrm{Alice}, \mathrm{Bob}\}, \quad C_2 = \{\mathrm{Carol}, \mathrm{Dave}, \mathrm{Eve}\}, \quad C_3 = \{\mathrm{Bob}, \mathrm{Carol}\}.$$

Next, we group these committees into two divisions (2-supervertices in $\mathcal{P}^2(V_0)$):

$$D_1 = \{C_1, C_2\}, \quad D_2 = \{C_2, C_3\}.$$

Define the 2-SuperHyperGraph $\mathrm{SHT}^{(2)} = (V, E)$ by

$$V = \{D_1, D_2\}, \qquad E = \big\{\{D_1, D_2\}\big\}.$$

Here, the single hyperedge $\{D_1, D_2\} \in E$ represents a cross-divisional task force that connects both divisions D_1 and D_2. Thus $\mathrm{SHT}^{(2)}$ models a three-layer hierarchy—employees → committees → divisions—and captures both intra-division and inter-division collaborations in one unified structure.

2.3 Molecular Graph

A molecular graph is a labeled graph representing atoms as vertices and covalent bonds as edges with specified bond types (cf. [52, 57, 63, 122]). The definition and example of a Molecular Graph are presented below.

Definition 2.21 (Molecular Graph)**.** [63] A *molecular graph* is a labeled simple graph

$$G = \big(V,\ E,\ \ell_V,\ \ell_E\big)$$

where

- V is a finite set of *atoms*;
- $E \subseteq \big\{\{u, v\} \mid u, v \in V,\ u \neq v\big\}$ is the set of *bonds*;
- $\ell_V : V \to \{\mathrm{C}, \mathrm{H}, \mathrm{O}, \dots\}$ assigns to each vertex its atomic symbol;
- $\ell_E : E \to \{\text{single}, \text{double}, \text{triple}\}$ assigns to each edge its bond order.

Thus G encodes the connectivity of a molecule: vertices are atoms, edges are chemical bonds, and labels record atom types and bond multiplicities.

Example 2.22 (Benzene Molecule as a Molecular Graph)**.** A benzene molecule is an aromatic hydrocarbon with six carbon atoms in a hexagonal ring and alternating double bonds (cf. [19, 118]). Consider benzene, C_6H_6. We model it by

$$V = \{\, c_1, c_2, c_3, c_4, c_5, c_6,\ h_1, h_2, h_3, h_4, h_5, h_6\},$$

$$E = \big\{\{c_i, c_{i+1}\}\ (i = 1, \dots, 5),\ \{c_6, c_1\},\ \{c_i, h_i\}\ (i = 1, \dots, 6)\big\}.$$

Label functions are

$$\ell_V(c_i) = \text{“C”}, \quad \ell_V(h_i) = \text{“H”},$$

$$\ell_E(\{c_i, c_{i+1}\}) = \begin{cases} \text{“double”}, & i \equiv 1, 3, 5 \pmod 2, \\ \text{“single”}, & i \equiv 0, 2, 4 \pmod 2, \end{cases} \qquad \ell_E(\{c_i, h_i\}) = \text{“single”}.$$

This graph G faithfully represents benzene's ring of alternating single and double C–C bonds and the six C–H bonds.

The conceptual diagram is shown in Figure 1.

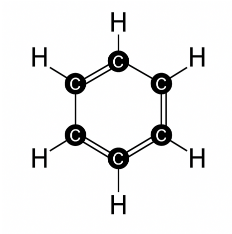

Figure 1: Hypergraph representation

3 Molecular Hypergraph

A Molecular Hypergraph represents molecules where vertices are atoms and hyperedges denote multi-atom interactions or molecular substructures [17, 61, 91]. The definition of a Molecular Hypergraph is presented as follows.

Definition 3.1 (Molecular Hypergraph)**.** [28] A *molecular hypergraph* is a node- and hyperedge-labeled hypergraph that models the atomic and bonding structure of a molecule. Formally, a molecular hypergraph

$$H = \big(V_H,\ E_H,\ \ell_V^H,\ \ell_E^H\big)$$

consists of:

- V_H a finite set of *nodes*, each representing a chemical bond;
- $E_H \subseteq \mathcal{P}(V_H)$ a finite set of *hyperedges*, where each hyperedge $e \in E_H$ is a subset of V_H corresponding to all bonds incident to a single atom;
- $\ell_V^H : V_H \to L_V^H$ a *node-labeling* function, assigning to each bond–node its bond type (e.g. single, double, triple);
- $\ell_E^H : E_H \to L_E^H$ a *hyperedge-labeling* function, assigning to each atom–hyperedge its atomic symbol or property (e.g. C, O, H).

This structure thus captures molecules at two hierarchical levels: bonds as nodes and atoms as hyperedges

Example 3.2 (Water Molecule as a Molecular Hypergraph)**.** A water molecule consists of two hydrogen atoms and one oxygen atom, forming a bent structure with polar covalent bonds (cf. [54, 76]). Consider the water molecule H_2O. We represent its two O–H bonds as nodes and its three atoms as hyperedges:

$$V_H = \{\, b_1, b_2\}, \quad E_H = \{\, e_O,\ e_{H_1},\ e_{H_2}\},$$

where

$$b_1 = \text{bond between O and } H_1, \quad b_2 = \text{bond between O and } H_2,$$

and the hyperedges are

$$e_O = \{\, b_1, b_2\}, \quad e_{H_1} = \{\, b_1\}, \quad e_{H_2} = \{\, b_2\}.$$

Labeling functions assign:

$$\ell_V^H(b_1) = \ell_V^H(b_2) = \text{“single”}, \quad \ell_E^H(e_O) = \text{“Oxygen”}, \quad \ell_E^H(e_{H_1}) = \ell_E^H(e_{H_2}) = \text{“Hydrogen”}.$$

Thus $H = (V_H, E_H, \ell_V^H, \ell_E^H)$ encodes the H_2O molecule: bonds are nodes, atoms are hyperedges connecting exactly those bonds incident to each atom. This concrete construction illustrates how molecular hypergraphs faithfully represent real chemical structures.

Example 3.3 (Benzene Molecule (C_6H_6) as a Molecular Hypergraph)**.** Consider the benzene molecule, C_6H_6. We represent its twelve covalent bonds as nodes and its twelve atoms as hyperedges:

$$V_H = \{\, b_1, b_2, b_3, b_4, b_5, b_6, b_7, b_8, b_9, b_{10}, b_{11}, b_{12}\},$$

where

$$\begin{aligned}
b_1 &= \text{bond between } C_1 \text{ and } C_2, & b_7 &= \text{bond between } C_1 \text{ and } H_1,\\
b_2 &= \text{bond between } C_2 \text{ and } C_3, & b_8 &= \text{bond between } C_2 \text{ and } H_2,\\
b_3 &= \text{bond between } C_3 \text{ and } C_4, & b_9 &= \text{bond between } C_3 \text{ and } H_3,\\
b_4 &= \text{bond between } C_4 \text{ and } C_5, & b_{10} &= \text{bond between } C_4 \text{ and } H_4,\\
b_5 &= \text{bond between } C_5 \text{ and } C_6, & b_{11} &= \text{bond between } C_5 \text{ and } H_5,\\
b_6 &= \text{bond between } C_6 \text{ and } C_1, & b_{12} &= \text{bond between } C_6 \text{ and } H_6.
\end{aligned}$$

The set of hyperedges is

$$\begin{aligned}
E_H = \{\, & e_{C_1}, e_{C_2}, e_{C_3}, e_{C_4}, e_{C_5}, e_{C_6},\\
& e_{H_1}, e_{H_2}, e_{H_3}, e_{H_4}, e_{H_5}, e_{H_6}\},
\end{aligned}$$

with

$$\begin{aligned}
e_{C_i} &= \{\, b_i,\ b_{i\oplus 1},\ b_{6+i}\,\}, \quad (i = 1, \ldots, 6),\\
e_{H_j} &= \{\, b_{6+j}\,\}, \quad (j = 1, \ldots, 6),
\end{aligned}$$

where $i \oplus 1$ is taken modulo 6 (so $6 \oplus 1 = 1$).

Labeling functions are given by

$$\ell_V^H(b_k) = \begin{cases} \text{“double”}, & k = 1, 3, 5,\\ \text{“single”}, & k = 2, 4, 6, 7, 8, 9, 10, 11, 12, \end{cases}$$

$$\ell_E^H(e_{C_i}) = \text{“Carbon”}, \quad \ell_E^H(e_{H_j}) = \text{“Hydrogen”}.$$

Thus

$$H = (V_H,\, E_H,\, \ell_V^H,\, \ell_E^H)$$

encodes the benzene molecule: bonds are nodes labeled by bond order, and atoms are hyperedges connecting exactly those bonds incident to each atom. This construction captures benzene's aromatic ring and hydrogen attachments in the molecular hypergraph framework.

Example 3.4 (Acetic Acid (CH_3COOH) as a Molecular Hypergraph)**.** Acetic acid consists of two carbon atoms, four hydrogen atoms, and two oxygen atoms, with the structural formula CH_3–COOH (cf. [59,64,115]). We represent its seven covalent bonds as nodes and its eight atoms as hyperedges:

$$V_H = \{\, b_1, b_2, b_3, b_4, b_5, b_6, b_7 \},$$

where

$$\begin{aligned} b_1 &= \text{bond } \mathrm{C_1{-}C_2}, & b_5 &= \text{double bond } \mathrm{C_2{-}O_1}, \\ b_2 &= \text{bond } \mathrm{C_1{-}H_1}, & b_6 &= \text{single bond } \mathrm{C_2{-}O_2}, \\ b_3 &= \text{bond } \mathrm{C_1{-}H_2}, & b_7 &= \text{bond } \mathrm{O_2{-}H_4}, \\ b_4 &= \text{bond } \mathrm{C_1{-}H_3}. \end{aligned}$$

The set of hyperedges is

$$E_H = \{\, e_{C_1}, e_{C_2}, e_{O_1}, e_{O_2}, e_{H_1}, e_{H_2}, e_{H_3}, e_{H_4} \},$$

with

$$\begin{aligned} e_{C_1} &= \{b_1, b_2, b_3, b_4\}, \\ e_{C_2} &= \{b_1, b_5, b_6\}, \\ e_{O_1} &= \{b_5\}, \\ e_{O_2} &= \{b_6, b_7\}, \\ e_{H_i} &= \{\, b_{i+1} \}, \quad i = 1, 2, 3, \\ e_{H_4} &= \{b_7\}. \end{aligned}$$

Labeling functions are defined by

$$\ell_V^H(b_k) = \begin{cases} \text{“double”}, & k = 5, \\ \text{“single”}, & k \neq 5, \end{cases} \qquad \ell_E^H(e_X) = \begin{cases} \text{“C”}, & X = C_1, C_2, \\ \text{“O”}, & X = O_1, O_2, \\ \text{“H”}, & X = H_1, \dots, H_4. \end{cases}$$

Thus

$$H = (V_H, E_H, \ell_V^H, \ell_E^H)$$

encodes the molecular hypergraph of acetic acid, with bonds as nodes labeled by bond order and atoms as hyperedges connecting exactly those bonds incident to each atom.

4 Molecular n-SuperHypergraph

A Molecular n-SuperHypergraph models hierarchical molecular structures using nested sets of atoms or interactions up to depth n. The definition of a Molecular n-SuperHyperGraph is presented as follows.

Definition 4.1 (Molecular n-SuperHyperGraph)**.** [28]
Let V_0 be a finite set of *bond identifiers* in a molecule. Define the n-th iterated powerset by

$$\mathcal{P}^0(V_0) = V_0, \qquad \mathcal{P}^{k+1}(V_0) = \mathcal{P}\big(\mathcal{P}^k(V_0)\big) \quad (k \geq 0),$$

where $\mathcal{P}(\cdot)$ is the usual powerset operation. A *molecular n-SuperHyperGraph* is then an ordered quadruple

$$H \;=\; \big(V_H,\; E_H,\; \ell_V^H,\; \ell_E^H\big)$$

with

$$V_H \;\subseteq\; \mathcal{P}^n(V_0), \quad E_H \;\subseteq\; \mathcal{P}^n(V_0),$$

where

- each element of V_H is called an *n-supernode*, representing a collection of bonds (possibly nested up to level n);
- each element of E_H is called an *n-superedge*, representing an atom or functional group connecting those supernodes;
- $\ell_V^H : V_H \to L_V$ labels each supernode by its bond-type or functional-group name;
- $\ell_E^H : E_H \to L_E$ labels each superedge by its atomic symbol or molecular fragment name.

This structure generalizes the molecular hypergraph ($n = 0$) and the molecular superhypergraph ($n = 1$) to arbitrary depth n.

Many examples of Molecular n-SuperHyperGraphs are presented below.

Example 4.2 (Ethanol (C_2H_5OH) as a Molecular 2-SuperHyperGraph)**.** Ethanol is a volatile, flammable alcohol with the formula C_2H_5OH, commonly used in beverages, fuel, and disinfectants (cf. [48, 109]). Let the base set of bonds be

$$V_0 = \{\, b_{\text{C–C}},\ b_{\text{C–H1}},\ b_{\text{C–H2}},\ b_{\text{C–H3}},\ b_{\text{C–H4}},\ b_{\text{C–H5}},\ b_{\text{C–O}},\ b_{\text{O–H}} \,\}.$$

Define two first-level subsets (functional groups):

$$F_{\text{ethyl}} = \{\, b_{\text{C–C}},\ b_{\text{C–H1}},\ b_{\text{C–H2}},\ b_{\text{C–H3}},\ b_{\text{C–H4}},\ b_{\text{C–H5}} \,\}, \quad F_{\text{hydroxyl}} = \{\, b_{\text{C–O}},\ b_{\text{O–H}} \,\}.$$

Form two second-level supernodes in $\mathcal{P}^2(V_0)$:

$$v_1 = \{\, F_{\text{ethyl}} \,\}, \qquad v_2 = \{\, F_{\text{hydroxyl}} \,\}.$$

Then the molecular 2-SuperHyperGraph for ethanol is

$$V_H = \{\, v_1,\ v_2\}, \quad E_H = \big\{\{\, v_1,\ v_2\}\big\},$$

with labeling functions

$$\ell_V^H(v_1) = \text{“Ethyl-group bonds”}, \quad \ell_V^H(v_2) = \text{“Hydroxyl-group bonds”},$$

$$\ell_E^H\big(\{\, v_1, v_2\}\big) = \text{“Ethanol molecule”}.$$

Here:

- $v_1, v_2 \in \mathcal{P}^2(V_0)$ are second-level supernodes each containing one functional-group subset;
- the single superedge $\{v_1, v_2\}$ connects them, representing the full C_2H_5OH structure;
- labels record the chemical interpretation at each hierarchy: bond collections $\to$ functional groups $\to$ whole molecule.

This example illustrates how a molecular 2-SuperHyperGraph encodes both bond-level and group-level organization in a real chemical species.

Example 4.3 (Acetic Acid (CH_3COOH) as a Molecular 2-SuperHyperGraph)**.** Acetic acid is a weak organic acid with formula CH_3COOH, responsible for vinegar's sour taste and strong smell (cf. [59, 64, 115]). Let the base set of bonds be

$$V_0 = \{b_1 = \mathrm{C_1–C_2},\ b_2 = \mathrm{C_1–H_1},\ b_3 = \mathrm{C_1–H_2},\ b_4 = \mathrm{C_1–H_3},$$

$$b_5 = \mathrm{C_2}{=}O_1,\ b_6 = \mathrm{C_2–O_2},\ b_7 = \mathrm{O_2–H}\}.$$

First-level functional groups (1-supernodes in $\mathcal{P}^1(V_0)$) are

$$F_{\text{methyl}} = \{\, b_1, b_2, b_3, b_4 \,\}, \quad F_{\text{carboxyl}} = \{\, b_5, b_6, b_7 \,\}.$$

Form the second-level supernodes in $\mathcal{P}^2(V_0)$:

$$v_1 = \{ F_{\text{methyl}} \}, \quad v_2 = \{ F_{\text{carboxyl}} \}.$$

Then the molecular 2-SuperHyperGraph for acetic acid is

$$V_H = \{ v_1, v_2 \}, \qquad E_H = \big\{ \{ v_1, v_2 \} \big\}.$$

Labeling functions are defined by

$$\ell_V^H(v_1) = \text{“Methyl-group bonds”}, \quad \ell_V^H(v_2) = \text{“Carboxyl-group bonds”},$$

$$\ell_E^H\big(\{v_1, v_2\}\big) = \text{“Acetic acid molecule”}.$$

Here:

- $v_1, v_2 \in \mathcal{P}^2(V_0)$ are second-level supernodes each containing one functional-group subset;
- the single superedge $\{v_1, v_2\}$ connects the methyl and carboxyl groups, representing the full CH_3COOH structure;
- labels record the chemical interpretation at each hierarchy: $\underbrace{\text{individual bonds}}_{\mathcal{P}^0(V_0)} \to \underbrace{\text{functional groups}}_{\mathcal{P}^1(V_0)} \to \underbrace{\text{whole molecule}}_{\mathcal{P}^2(V_0)}$.

This example demonstrates how a molecular 2-SuperHyperGraph encodes both bond-level and group-level organization in a real chemical species.

Example 4.4 (Ethyl Acetate ($CH_3COOCH_2CH_3$) as a Molecular 3-SuperHyperGraph)**.** Ethyl acetate is a colorless, sweet-smelling organic solvent with the formula $CH_3COOCH_2CH_3$, commonly used in paints and adhesives (cf. [74, 128]). Let the base set of bonds be

$$V_0 = \{b_1 = \mathrm{C}_1{-}O,\ b_2 = \mathrm{O}{-}\mathrm{C}_2,\ b_3 = \mathrm{C}_2{-}\mathrm{C}_3,\ b_4 = \mathrm{C}_3{-}\mathrm{H}_1,\ b_5 = \mathrm{C}_3{-}\mathrm{H}_2,\ b_6 = \mathrm{C}_3{-}\mathrm{H}_3\}.$$

First-level functional groups (1-supernodes in $\mathcal{P}^1(V_0)$) are

$$F_{\text{acetyl}} = \{ b_1,\ b_2 \}, \quad F_{\text{ethyl}} = \{ b_3,\ b_4,\ b_5,\ b_6 \}.$$

Second-level moieties (2-supernodes in $\mathcal{P}^2(V_0)$) are

$$M_{\text{acetyl}} = \{ F_{\text{acetyl}} \}, \quad M_{\text{ethyl}} = \{ F_{\text{ethyl}} \}.$$

Third-level supernodes (3-supernodes in $\mathcal{P}^3(V_0)$) are

$$U_1 = \{ M_{\text{acetyl}} \}, \quad U_2 = \{ M_{\text{ethyl}} \}.$$

Then the molecular 3-SuperHyperGraph for ethyl acetate is defined by

$$V_H = \{ U_1,\ U_2 \}, \quad E_H = \big\{ \{ U_1,\ U_2 \} \big\}.$$

Labeling functions assign:

$$\ell_V^H(U_1) = \text{“Acetyl moiety”}, \quad \ell_V^H(U_2) = \text{“Ethyl moiety”}, \quad \ell_E^H\big(\{U_1, U_2\}\big) = \text{“Ethyl acetate molecule”}.$$

In this construction:

- Bonds ($\mathcal{P}^0$) form functional groups ($\mathcal{P}^1$),
- which form moieties ($\mathcal{P}^2$),
- which in turn form supernodes at level 3 ($\mathcal{P}^3$),

- and a single superedge connects them to represent the entire molecule.

Thus the 3-SuperHyperGraph captures bond-level, group-level, moiety-level, and full-molecule structure in one unified framework.

Example 4.5 (Aspirin ($C_9H_8O_4$) as a Molecular 3-SuperHyperGraph)**.** Aspirin is a widely used medication with formula $C_9H_8O_4$, known for relieving pain, fever, and inflammation (cf. [11, 110, 116]). Let the base set of bonds be

$$V_0 = \{b_1 = \mathrm{C}_1{-}\mathrm{C}_2,\ b_2 = \mathrm{C}_2{-}\mathrm{C}_3,\ b_3 = \mathrm{C}_3{-}\mathrm{C}_4,\ b_4 = \mathrm{C}_4{-}\mathrm{C}_5,\ b_5 = \mathrm{C}_5{-}\mathrm{C}_6,\ b_6 = \mathrm{C}_6{-}\mathrm{C}_1,\ b_7 = \mathrm{C}_1{-}\mathrm{C}_7,$$

$$b_8 = \mathrm{C}_7{=}O_8,\ b_9 = \mathrm{C}_7{-}O_9,\ b_{10} = O_9{-}H_{10}, b_{11} = \mathrm{C}_2{-}O_{11},$$

$$b_{12} = O_{11}{-}\mathrm{C}_8,\ b_{13} = \mathrm{C}_8{-}H_{11},\ b_{14} = \mathrm{C}_8{-}H_{12},\ b_{15} = \mathrm{C}_8{-}H_{13}\}.$$

First-level functional groups (1-supernodes in $\mathcal{P}^1(V_0)$) are

$$F_{\text{ring}} = \{b_1, b_2, b_3, b_4, b_5, b_6\}, \quad F_{\text{carboxyl}} = \{b_7, b_8, b_9, b_{10}\}, \quad F_{\text{ester}} = \{b_{11}, b_{12}, b_{13}, b_{14}, b_{15}\}.$$

Second-level moieties (2-supernodes in $\mathcal{P}^2(V_0)$) are

$$M_{\text{salicylic}} = \{\, F_{\text{ring}},\ F_{\text{carboxyl}} \,\}, \quad M_{\text{acetyl}} = \{\, F_{\text{ester}} \,\}.$$

Third-level supernodes (3-supernodes in $\mathcal{P}^3(V_0)$) are

$$U_1 = \{\, M_{\text{salicylic}} \,\}, \quad U_2 = \{\, M_{\text{acetyl}} \,\}.$$

Then the molecular 3-SuperHyperGraph for aspirin is

$$V_H = \{\, U_1,\ U_2\}, \qquad E_H = \big\{\{\, U_1,\ U_2\}\big\}.$$

Labeling functions assign:

$$\ell_V^H(U_1) = \text{“Salicylic acid moiety”}, \quad \ell_V^H(U_2) = \text{“Acetyl moiety”}, \quad \ell_E^H\big(\{U_1, U_2\}\big) = \text{“Aspirin molecule”}.$$

In this framework:

- Bonds ($\mathcal{P}^0$) form functional groups ($\mathcal{P}^1$),
- Functional groups form moieties ($\mathcal{P}^2$),
- Moieties form supernodes at level 3 ($\mathcal{P}^3$),
- A single superedge connects the two level-3 nodes to represent the complete molecule.

Thus the 3-SuperHyperGraph captures bond-level, group-level, moiety-level, and whole-molecule structure in one unified model.

Example 4.6 (Ethylene Glycol ($HO–CH_2–CH_2–OH$) as a Molecular 3-SuperHyperGraph)**.** Ethylene glycol is a colorless, odorless liquid with formula $C_2H_6O_2$, commonly used as antifreeze and coolant in engines (cf. [72, 105, 123]). Let the base set of bonds (level 0) be

$$V_0 = \{b_1 = \mathrm{C}_1{-}\mathrm{C}_2,\ b_2 = \mathrm{C}_1{-}\mathrm{H}_1,\ b_3 = \mathrm{C}_1{-}\mathrm{H}_2,\ b_4 = \mathrm{C}_2{-}\mathrm{H}_3,\ b_5 = \mathrm{C}_2{-}\mathrm{H}_4,$$

$$b_6 = \mathrm{C}_1{-}\mathrm{O}_1,\ b_7 = \mathrm{O}_1{-}\mathrm{H}_5,\ b_8 = \mathrm{C}_2{-}\mathrm{O}_2,\ b_9 = \mathrm{O}_2{-}\mathrm{H}_6\}.$$

First-level functional groups (1-supernodes in $\mathcal{P}^1(V_0)$) are

$$F_1 = \{\, b_1, b_2, b_3\}, \quad F_2 = \{\, b_1, b_4, b_5\}, \quad F_3 = \{\, b_6, b_7\}, \quad F_4 = \{\, b_8, b_9\}.$$

Here F_1 and F_2 are the two *methylene* groups at C_1 and C_2, and F_3, F_4 are the two *hydroxyl* groups.

Second-level moieties (2-supernodes in $\mathcal{P}^2(V_0)$) are

$$M_1 = \{\, F_1, F_3\}, \quad M_2 = \{\, F_2, F_4\}.$$

Each M_i corresponds to a *hydroxymethyl* moiety at carbon i.

Third-level supernodes (3-supernodes in $\mathcal{P}^3(V_0)$) are

$$U_1 = \{ M_1\}, \quad U_2 = \{ M_2\}.$$

Finally, the molecular 3-SuperHyperGraph is

$$V_H = \{ U_1, U_2\}, \qquad E_H = \big\{\{ U_1, U_2\}\big\}.$$

Labeling functions assign:

$$\ell_V^H(U_1) = \text{“Hydroxymethyl moiety at C}_1\text{”}, \quad \ell_V^H(U_2) = \text{“Hydroxymethyl moiety at C}_2\text{”},$$

$$\ell_E^H\big(\{U_1, U_2\}\big) = \text{“Ethylene glycol molecule”}.$$

In this example:

- Level 0 captures each individual bond in the molecule.
- Level 1 groups bonds into methylene and hydroxyl functional groups.
- Level 2 assembles each carbon's methylene + hydroxyl into hydroxymethyl moieties.
- Level 3 creates supernodes for each hydroxymethyl moiety and a single superedge connecting them, representing the full ethylene glycol structure.

Example 4.7 (Penicillin G ($C_{16}H_{18}N_2O_4S$) as a Molecular 4-SuperHyperGraph)**.** Penicillin G is a natural antibiotic with formula $C_{16}H_{18}N_2O_4S$, effective against gram-positive bacteria and used intravenously (cf. [77, 84]). Let the base set of bonds (level 0) be

$$V_0 = \{b_1 = N_1 - C_2,\ b_2 = C_2 - C_3,\ b_3 = C_3 - C_4,\ b_4 = C_4 - N_1,\ b_5 = C_4 - C_5,\ b_6 = C_5 - S_6,$$

$$b_7 = S_6 – C_7,\ b_8 = C_7 – C_4, b_9 = N_1 – C_8,\ b_{10} = C_8 – C_9,\ b_{11} = C_9 – C_{10},\ b_{12} = C_{10} – C_{11},\ b_{13} = C_{11} – C_{12},\ b_{14} = C_{12} – C_9\}.$$

Form the functional groups (1-supernodes, level 1):

$$F_{\beta\text{-lactam}} = \{b_1, b_2, b_3, b_4\}, \quad F_{\text{thiazolidine}} = \{b_5, b_6, b_7, b_8\},$$

$$F_{\text{linkage}} = \{b_9\}, \quad F_{\text{phenyl}} = \{b_{10}, b_{11}, b_{12}, b_{13}, b_{14}\}.$$

Form the moieties (2-supernodes, level 2):

$$M_{\text{ring}} = \{F_{\beta\text{-lactam}},\ F_{\text{thiazolidine}}\}, \quad M_{\text{side}} = \{F_{\text{linkage}},\ F_{\text{phenyl}}\}.$$

Form the super-moieties (3-supernodes, level 3):

$$S_{\text{penam}} = \{ M_{\text{ring}} \}, \quad S_{\text{phenylacetyl}} = \{ M_{\text{side}} \}.$$

Finally, form the 4-supernodes (level 4):

$$U_1 = \{ S_{\text{penam}} \}, \quad U_2 = \{ S_{\text{phenylacetyl}} \}.$$

The molecular 4-SuperHyperGraph for Penicillin G is then

$$V_H = \{ U_1,\ U_2\}, \qquad E_H = \big\{\{ U_1,\ U_2\}\big\}.$$

Label functions assign:

$$\ell_V^H(U_1) = \text{“Penam core”}, \quad \ell_V^H(U_2) = \text{“Phenylacetyl side chain”}, \quad \ell_E^H(\{U_1, U_2\}) = \text{“Penicillin G molecule”}.$$

- *Level 0 (bonds)*: individual bond identifiers $b_1, \ldots, b_{14}$.
- *Level 1 (functional groups)*: β-lactam ring, thiazolidine ring, linkage bond, phenyl ring.

- *Level 2 (moieties)*: fused ring system M_{ring} and side-chain system M_{side}.
- *Level 3 (super-moieties)*: penam core S_{penam} and phenylacetyl branch $S_{\text{phenylacetyl}}$.
- *Level 4 (4-supernodes)*: top-level groupings U_1, U_2 representing the molecule's two principal parts.

This 4-SuperHyperGraph captures bond-level, group-level, moiety-level, super-moiety-level, and whole-molecule structure in one unified framework.

Example 4.8 (Estradiol ($C_{18}H_{24}O_2$) as a Molecular 4-SuperHyperGraph)**.** Estradiol is a primary female sex hormone with formula $C_{18}H_{24}O_2$, regulating reproductive and secondary sexual characteristics (cf. [78, 111]). Let the base set of bonds (level 0) be

$$V_0 = \{b_1 = C_1\text{–}C_2,\ b_2 = C_2\text{–}C_3,\ b_3 = C_3\text{–}C_4,\ b_4 = C_4\text{–}C_5,\ b_5 = C_5\text{–}C_6,\ b_6 = C_6\text{–}C_7,\ b_7 = C_7\text{–}C_8,\ b_8 = C_8\text{–}C_9,$$

$$b_9 = C_9\text{–}C_{10},\ b_{10} = C_{10}\text{–}C_5,\ b_{11} = C_8\text{–}C_{11},\ b_{12} = C_{11}\text{–}C_{12},\ b_{13} = C_{12}\text{–}C_{13},\ b_{14} = C_{13}\text{–}C_{14},\ b_{15} = C_{14}\text{–}C_{15},$$

$$b_{16} = C_{15}-C_8, b_{17} = C_3-O_1,\ b_{18} = C_{17}-O_2,\ b_{19} = O_2-H_{18}\}.$$

First-level functional groups (1-supernodes in $\mathcal{P}^1(V_0)$) are

$$F_A = \{b_1, b_2, b_3, b_4\}, \quad F_B = \{b_4, b_5, b_6, b_7\}, \quad F_C = \{b_7, b_8, b_{11}, b_{10}\},$$

$$F_D = \{b_{10}, b_9, b_8, b_6\}, F_{\text{OH-3}} = \{b_{17}\}, \quad F_{\text{OH-17}} = \{b_{18}, b_{19}\}.$$

Second-level moieties (2-supernodes in $\mathcal{P}^2(V_0)$) are

$$M_{\text{rings}} = \{F_A, F_B, F_C, F_D\},$$

$$M_{\text{hydroxyl}} = \{F_{\text{OH-3}},\ F_{\text{OH-17}}\}.$$

Third-level super-moieties (3-supernodes in $\mathcal{P}^3(V_0)$) are

$$S_{\text{core}} = \{\ M_{\text{rings}}\ \},$$

$$S_{\text{functional}} = \{\ M_{\text{hydroxyl}}\ \}.$$

Fourth-level supernodes (4-supernodes in $\mathcal{P}^4(V_0)$) are

$$U_1 = \{\ S_{\text{core}}\ \}, \quad U_2 = \{\ S_{\text{functional}}\ \}.$$

Then the molecular 4-SuperHyperGraph is

$$V_H = \{\ U_1,\ U_2\}, \qquad E_H = \big\{\{\ U_1,\ U_2\}\big\}.$$

Labeling functions assign:

$$\ell_V^H(U_1) = \text{“Steroid nucleus (rings A–D)”},$$

$$\ell_V^H(U_2) = \text{“Hydroxyl groups at C3 and C17”},$$

$$\ell_E^H(\{U_1, U_2\}) = \text{“Estradiol molecule”}.$$

This construction captures:

- *Level 0 (bonds)*: individual C–C, C–O, and O–H bonds;
- *Level 1 (functional groups)*: four fused rings A–D and two hydroxyl attachments;
- *Level 2 (moieties)*: the complete ring system vs. the hydroxyl functionalities;
- *Level 3 (super-moieties)*: core steroid framework vs. functional group assembly;
- *Level 4 (4-supernodes)*: top-level partition into nucleus and functional modules, connected by a single superedge representing the full Estradiol molecule.

Theorem 4.9 (Level-Flattening Theorem)**.** *Let $H = (V_H, E_H, \ell_V, \ell_E)$ be a molecular n-SuperHyperGraph over the base bond set V_0. For each k with $0 \le k \le n$, define the k*-flattening map

$$\varphi_k : \mathcal{P}^n(V_0) \longrightarrow \mathcal{P}^{n-k}(V_0), \qquad X \mapsto \bigcup_{Y \in X} Y,$$

applied recursively k times. Then

$$H^{(n-k)} \;=\; \big(\varphi_k(V_H),\ \varphi_k(E_H),\ \ell_V \circ \varphi_k,\ \ell_E \circ \varphi_k\big)$$

is a well-defined molecular $(n-k)$-SuperHyperGraph.

Proof. Since $V_H \subseteq \mathcal{P}^n(V_0)$ and $E_H \subseteq \mathcal{P}^n(V_0)$, applying φ_k yields $\varphi_k(V_H) \subseteq \mathcal{P}^{n-k}(V_0)$ and $\varphi_k(E_H) \subseteq \mathcal{P}^{n-k}(V_0)$. The composites $\ell_V \circ \varphi_k$ and $\ell_E \circ \varphi_k$ remain valid labeling functions (their codomains are unchanged). Thus all axioms of a molecular $(n-k)$-SuperHyperGraph hold by construction. In particular:

- The new vertex set is a collection of $(n-k)$-supernodes.
- The new edge set is a collection of $(n-k)$-superedges.
- Labels remain consistent under flattening.

Hence $H^{(n-k)}$ satisfies the definition of a molecular $(n-k)$-SuperHyperGraph. □

Theorem 4.10 (Connectivity Equivalence)**.** *Let H be a molecular n-SuperHyperGraph and let $H^{(0)}$ be its 0-flattening (the underlying molecular hypergraph). Then H is connected (in the sense that its primal graph is connected) if and only if $H^{(0)}$ is connected.*

Proof. Recall that the *primal graph $G(H)$* of a hypergraph H has the same vertex set, with an ordinary edge between two vertices whenever they appear together in some hyperedge. Under each flattening step φ_k, the condition "two $(n-k)$-supernodes appear in a common $(n-k)$-superedge" is exactly the image of "two n-supernodes appear in a common n-superedge." Hence adjacency relations in $G(H)$ are preserved through flattening down to $G(H^{(0)})$. Therefore any path in $G(H)$ projects to a path in $G(H^{(0)})$ and vice versa. Connectedness is thus equivalent at all levels. □

Theorem 4.11 (Bond-Coverage Theorem)**.** *In any molecular n-SuperHyperGraph H over base bond set V_0, every bond identifier $b \in V_0$ is covered by the union of the flattened superedges:*

$$\bigcup_{e \in E_H} \varphi_n(e) \;=\; V_0.$$

Proof. We prove by induction on n.

Base case $n = 0$: Then H is a molecular hypergraph (V_H, E_H) over V_0, and by definition of a molecular hypergraph each bond appears in at least one atomic hyperedge. Hence $\bigcup_{e \in E_H} e = V_0$.

Inductive step: Assume true for $n-1$. Let H be a molecular n-SHG. Form its 1-flattening H' which is a molecular $(n-1)$-SHG. By induction,

$$\bigcup_{e' \in E_{H'}} \varphi_{n-1}(e') = V_0$$

. But

$$E_{H'} = \varphi_1(E_H)$$

and

$$\varphi_{n-1} \circ \varphi_1 = \varphi_n$$

. Therefore

$$\bigcup_{e \in E_H} \varphi_n(e) \;=\; \bigcup_{e' \in E_{H'}} \varphi_{n-1}(e') \;=\; V_0.$$

This completes the induction. □

Theorem 4.12 (Induced Sub-SuperHyperGraph Theorem)**.** *Let $H = (V_H, E_H, \ell_V, \ell_E)$ be a molecular n-SuperHyperGraph over base bond set V_0, and let $B \subseteq V_0$ be any nonempty subset of bonds. Define*

$$V' = \{\, v \in V_H : v \subseteq \mathcal{P}^n(B)\,\}, \quad E' = \{\, e \in E_H : e \subseteq \mathcal{P}^n(B)\,\}.$$

Then

$$H[B] = (V', E',\ \ell_V|_{V'},\ \ell_E|_{E'})$$

is itself a well-defined molecular n-SuperHyperGraph over B.

Proof. Since $V_H \subseteq \mathcal{P}^n(V_0)$, any $v \in V_H$ satisfying $v \subseteq \mathcal{P}^n(B)$ must lie in $\mathcal{P}^n(B)$. Hence $V' \subseteq \mathcal{P}^n(B)$. Similarly $E' \subseteq \mathcal{P}^n(B)$. The restricted labeling functions $\ell_V|_{V'}$ and $\ell_E|_{E'}$ still map into the same label sets and assign the same chemical interpretations. All defining axioms of an n-SuperHyperGraph hold on V', E' by closure under subset, so $H[B]$ is a molecular n-SuperHyperGraph over the smaller bond set B. □

Theorem 4.13 (Label-Preservation Under Flattening)**.** *Let H be a molecular n-SuperHyperGraph and let φ_k be the k-flattening map from level n to $n-k$. Then for every supernode $v \in V_H$,*

$$\ell_V(v) \ = \ \ell_V\big(\varphi_k(v)\big),$$

and similarly $\ell_E(e) = \ell_E(\varphi_k(e))$ for every superedge $e \in E_H$. In other words, flattening does not alter any labels.

Proof. By definition of φ_k, we have $\varphi_k : \mathcal{P}^n(V_0) \to \mathcal{P}^{n-k}(V_0)$ and labels are assigned only by the map ℓ_V or ℓ_E on the original set elements. Because ℓ_V and ℓ_E depend solely on the chemical identity of the collection (and not on its nesting depth), applying φ_k does not change the underlying set whose label is being queried. Hence $\ell_V(v) = \ell_V(\varphi_k(v))$ and likewise for ℓ_E. □

Theorem 4.14 (Atomic-Degree Bound Theorem)**.** *Let H be a molecular n-SuperHyperGraph, and let $G(H)$ be its primal graph on supernodes V_H. Then for any supernode $v \in V_H$,*

$$\deg_{G(H)}(v) \ \leq \ \big|\{\, e \in E_H : v \subseteq e\}\big| \ \times (|e| - 1),$$

where $|e|$ is the cardinality of the superedge e. In particular, each supernode's degree is bounded by the number and sizes of superedges containing it.

Proof. By construction, $G(H)$ connects two distinct supernodes v, w whenever there exists some superedge $e \in E_H$ with $\{v, w\} \subseteq e$. Fix v. For each superedge e containing v, v acquires edges in $G(H)$ to each of the other $|e| - 1$ nodes in e. Summing over all such e yields the stated bound. Since an edge in $G(H)$ may be counted multiple times if two superedges share the same pair $\{v, w\}$, this is an upper bound. □

Theorem 4.15 (Hierarchical Partition Refinement)**.** *In a molecular n-SuperHyperGraph H, the collection of supernodes at level k $\varphi_{n-k}(V_H) \subseteq \mathcal{P}^k(V_0)$ forms a partition of V_0 that refines the partition obtained at level $k-1$. That is, every k-flattened supernode is contained in exactly one $(k-1)$-flattened supernode.*

Proof. Level n-supernodes $V_H \subseteq \mathcal{P}^n(V_0)$ cover V_0 by the Bond-Coverage Theorem. Applying φ_{n-k} yields $\varphi_{n-k}(V_H) \subseteq \mathcal{P}^k(V_0)$. Since $\bigcup_{v \in V_H} \varphi_n(v) = V_0$ and each v flattens to a unique set in $\mathcal{P}^0(V_0)$, the families at intermediate levels cover V_0 without overlap beyond set-inclusion. Moreover, if $X \in \varphi_{n-k}(V_H)$ and $Y \in \varphi_{n-(k-1)}(V_H)$, then $X \subseteq Y$ by the recursive definition of φ. Hence the k-level partition refines the $(k-1)$-level partition. □

5 Conclusion and Future Works

This paper has examined the formal definitions, illustrative examples, and structural properties of *Molecular Hypergraphs* and *Molecular n-SuperHypergraphs*, providing a rigorous foundation for modeling hierarchical biochemical interactions. We hope that future work will further advance experimental, mathematical, and chemical investigations into these frameworks.

As part of our future research agenda, we intend to explore extensions of the Molecular Hypergraph and Molecular n-SuperHypergraph frameworks by integrating advanced uncertainty-handling methodologies. These include Fuzzy Sets [124, 125], Intuitionistic Fuzzy Sets [9, 10], Vague Sets [5, 47], Rough Sets [87, 88], Bipolar Fuzzy Sets [4], HyperFuzzy Sets [29, 60, 104], Picture Fuzzy Sets [20, 55], Hesitant Fuzzy Sets [106, 107], and Neutrosophic Sets [98, 103].

We also plan to investigate their more recent extensions, such as Quadripartitioned Neutrosophic Sets [44, 65, 121], Plithogenic Sets [35, 41, 42], and HyperPlithogenic Sets [36–38]. These integrations aim to enrich the expressive power of the models and extend their applicability to increasingly complex and hierarchically uncertain systems in both theoretical and applied domains.

Furthermore, as a future direction, we hope to explore extended concepts of the present paper by incorporating structures such as directed graphs [32], bidirected graphs [14, 49, 120], and multidirected graphs [**?**, 85].

Author Contributions

The paper has been solely authored by the corresponding author at this stage.

Data Availability

This research is purely theoretical, involving no data collection or analysis. We encourage future researchers to pursue empirical investigations to further develop and validate the concepts introduced here.

Disclaimer (Artificial intelligence)

Option 1:
Author(s) hereby declare that NO generative AI technologies such as Large Language Models (ChatGPT, COPILOT, etc.) and text-to-image generators have been used during the writing or editing of this manuscript.

Study Limitations

The theoretical concepts presented in this paper have not yet been subject to practical implementation or empirical validation. Future researchers are invited to explore these ideas in applied or experimental settings. Although every effort has been made to ensure the accuracy of the content and the proper citation of sources, unintentional errors or omissions may persist. Readers should independently verify any referenced materials.

To the best of the authors' knowledge, all mathematical statements and proofs contained herein are correct and have been thoroughly vetted. Should you identify any potential errors or ambiguities, please feel free to contact the authors for clarification.

The results presented are valid only under the specific assumptions and conditions detailed in the manuscript. Extending these findings to broader mathematical structures may require additional research. The opinions and conclusions expressed in this work are those of the authors alone and do not necessarily reflect the official positions of their affiliated institutions.

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