
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. A *hypergraph* generalizes the concept of a traditional graph by allowing edges—called *hyperedges*—to connect more than two vertices simultaneously [9]. A *superhypergraph* further extends this idea by incorporating recursively defined powerset layers, enabling hierarchical and self-referential relationships among hyperedges [80].

This paper investigates the formalization, illustrative examples, and structural properties of *molecular hypergraphs* and *molecular superhypergraphs* (cf. [21]). 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

Graph theory is a branch of mathematics that studies the properties of networks, where nodes (called vertices) are connected by links (called edges) [15, 16]. Graphs have been extensively studied for applications in various fields such as social science [57, 72], graph neural networks (GNNs) [4, 29, 106], and network analysis [59, 61].

Mathematical structures can often be extended into hyperstructures and superhyperstructures by utilizing the power set and n -th iterated powerset constructions (cf. [12, 44, 81]). 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 [9, 10]. A superhypergraph takes this further by employing recursively nested powerset structures, enabling hierarchical and self-similar relationships among hyperedges themselves [32, 79].

Chemistry is the scientific study of matter, including its properties, structure, composition, and interactions [20, 71]. Graphs are widely used in the field of chemistry to represent and analyze molecular structures [8, 17, 58]. Several types of graphs—such as *molecular graphs* [38, 48, 56, 105] and *pharmacophore graphs* [76, 99]—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 [24, 37, 88, 94]. 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 [51, 52].

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. [21]). Through these generalizations, we aim to contribute to the advancement of hierarchical modeling in chemistry, providing new perspectives on complex molecular structures.

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 [82]. Intuitively, the n -th powerset is a repeated application of the powerset operation. Relevant definitions and simple examples are provided below.

Definition 2.1 (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 2.2 (Powerset). [25, 75] 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:

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

Definition 2.3 (n -th Powerset). (cf. [21, 25, 77, 82])

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.

Definition 2.4 (Classical Structure). (cf. [77, 82]) 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:

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

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 2.5 (Hyperoperation). (cf. [92, 93]) 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:

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

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

Definition 2.6 (Hyperstructure). (cf. [25, 82]) 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.

Definition 2.7 (SuperHyperOperations). (cf. [82]) 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:

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

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 2.8 (n -Superhyperstructure). (cf. [23, 26, 82]) 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 2.9 (Smartphone Product Bundling as a 2-Superhyperstructure). (cf. [74]) Let the base set of components be

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

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

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

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

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

by

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

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

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 [9, 19, 41, 42]. 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 [1, 35, 66, 68].

Definition 2.10 (Hypergraph). [9, 10] 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.

Definition 2.11 (n-SuperHyperGraph). [27, 31, 79, 80]

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

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

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 2.12 (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. [18, 97]). Let $V_0 = \{\text{Alice, Bob, Carol, Dave, Eve}\}$ be the set of individual employees in a company. We first form the following committees (1-supervertices in $\mathcal{P}^1(V_0)$):

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

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 $\text{SHT}^{(2)} = (V, E)$ by

$$V = \{D_1, D_2\}, \quad E = \{\{D_1, D_2\}\}.$$

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 $\text{SHT}^{(2)}$ models a three-layer hierarchy—employees \rightarrow committees \rightarrow 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. [43, 47, 53, 101]).

Definition 2.13 (Molecular Graph). [53] A *molecular graph* is a labeled simple graph

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

where

- V is a finite set of *atoms*;
- $E \subseteq \{\{u, v\} \mid u, v \in V, u \neq v\}$ is the set of *bonds*;
- $\ell_V : V \rightarrow \{\text{C, H, O, } \dots\}$ assigns to each vertex its atomic symbol;
- $\ell_E : E \rightarrow \{\text{single, double, triple}\}$ 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 2.14 (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. [13,98]). Consider benzene, C_6H_6 . We model it by

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

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

Label functions are

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

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

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

3 Molecular Hypergraph

A Molecular Hypergraph represents molecules where vertices are atoms and hyperedges denote multi-atom interactions or molecular substructures [11,51,73]. The definition of a Molecular Hypergraph is presented as follows.

Definition 3.1 (Molecular Hypergraph). [21] A *molecular hypergraph* is a node- and hyperedge-labeled hypergraph that models the atomic and bonding structure of a molecule. Formally, a molecular hypergraph

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

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;
- $\ell_V^H : V_H \rightarrow L_V^H$ a *node-labeling* function, assigning to each bond–node its bond type (e.g. single, double, triple);
- $\ell_E^H : E_H \rightarrow L_E^H$ 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. [45,63]). 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

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

with

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

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

Labeling functions are given by

$$\begin{aligned} \ell_V^H(b_k) &= \begin{cases} \text{"double"}, & k = 1, 3, 5, \\ \text{"single"}, & k = 2, 4, 6, 7, 8, 9, 10, 11, 12, \end{cases} \\ \ell_E^H(e_{C_i}) &= \text{"Carbon"}, \quad \ell_E^H(e_{H_j}) = \text{"Hydrogen"}. \end{aligned}$$

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.

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). [21]

Let V_0 be a finite set of *bond identifiers* in a molecule. Define the n -th iterated powerset by

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

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

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

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;
- $\ell_V^H : V_H \rightarrow L_V$ labels each supernode by its bond-type or functional-group name;
- $\ell_E^H : E_H \rightarrow L_E$ 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. [40, 89]). Let the base set of bonds be

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

Define two first-level subsets (functional groups):

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

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

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

Then the molecular 2-SuperHyperGraph for ethanol is

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

with labeling functions

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

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

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 \rightarrow functional groups \rightarrow 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. [49, 54, 95]). Let the base set of bonds be

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

$$b_5 = C_2=O_1, b_6 = C_2-O_2, b_7 = O_2-H \}.$$

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

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

Labeling functions are defined by

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

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

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: $\underbrace{\text{individual bonds}}_{\mathcal{P}^0(V_0)} \rightarrow \underbrace{\text{functional groups}}_{\mathcal{P}^1(V_0)} \rightarrow \underbrace{\text{whole molecule}}_{\mathcal{P}^2(V_0)}.$

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 ($\text{CH}_3\text{COOCH}_2\text{CH}_3$) as a Molecular 3-SuperHyperGraph). Ethyl acetate is a colorless, sweet-smelling organic solvent with the formula $\text{CH}_3\text{COOCH}_2\text{CH}_3$, commonly used in paints and adhesives (cf. [62, 107]). Let the base set of bonds be

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

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

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

Labeling functions assign:

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

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. [7, 90, 96]). Let the base set of bonds be

$$V_0 = \{b_1 = C_1-C_2, b_2 = C_2-C_3, b_3 = C_3-C_4, b_4 = C_4-C_5, b_5 = C_5-C_6, b_6 = C_6-C_1, b_7 = C_1-C_7, \\ b_8 = C_7=O_8, b_9 = C_7-O_9, b_{10} = O_9-H_{10}, b_{11} = C_2-O_{11}, b_{12} = O_{11}-C_8, b_{13} = C_8-H_{11}, b_{14} = C_8-H_{12}, b_{15} = C_8-H_{13}\}.$$

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

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

Labeling functions assign:

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

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. [60, 85, 102]). Let the base set of bonds (level 0) be

$$V_0 = \{b_1 = C_1-C_2, b_2 = C_1-H_1, b_3 = C_1-H_2, b_4 = C_2-H_3, b_5 = C_2-H_4, \\ b_6 = C_1-O_1, b_7 = O_1-H_5, b_8 = C_2-O_2, b_9 = O_2-H_6\}.$$

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

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

Labeling functions assign:

$$\begin{aligned} \ell_V^H(U_1) &= \text{“Hydroxymethyl moiety at C}_1\text{”}, & \ell_V^H(U_2) &= \text{“Hydroxymethyl moiety at C}_2\text{”}, \\ \ell_E^H(\{U_1, U_2\}) &= \text{“Ethylene glycol molecule”}. \end{aligned}$$

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. [64, 67]). Let the base set of bonds (level 0) be

$$\begin{aligned} V_0 = \{ & b_1 = N_1-C_2, b_2 = C_2-C_3, b_3 = C_3-C_4, b_4 = C_4-N_1, b_5 = C_4-C_5, b_6 = C_5-S_6, \\ & b_7 = S_6-C_7, b_8 = C_7-C_4, b_9 = N_1-C_8, b_{10} = C_8-C_9, b_{11} = C_9-C_{10}, b_{12} = C_{10}-C_{11}, b_{13} = C_{11}-C_{12}, b_{14} = C_{12}-C_9 \}. \end{aligned}$$

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

$$\begin{aligned} F_{\beta\text{-lactam}} &= \{b_1, b_2, b_3, b_4\}, & F_{\text{thiazolidine}} &= \{b_5, b_6, b_7, b_8\}, \\ F_{\text{linkage}} &= \{b_9\}, & F_{\text{phenyl}} &= \{b_{10}, b_{11}, b_{12}, b_{13}, b_{14}\}. \end{aligned}$$

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

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

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, \dots, 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. [65,91]). Let the base set of bonds (level 0) be

$$V_0 = \{b_1 = C_1-C_2, b_2 = C_2-C_3, b_3 = C_3-C_4, b_4 = C_4-C_5, b_5 = C_5-C_6, b_6 = C_6-C_7, b_7 = C_7-C_8, b_8 = C_8-C_9, \\ b_9 = C_9-C_{10}, b_{10} = C_{10}-C_5, b_{11} = C_8-C_{11}, b_{12} = C_{11}-C_{12}, b_{13} = C_{12}-C_{13}, b_{14} = C_{13}-C_{14}, b_{15} = C_{14}-C_{15}, \\ b_{16} = C_{15}-C_8, b_{17} = C_3-O_1, b_{18} = C_{17}-O_2, b_{19} = O_2-H_{18}\}.$$

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

$$F_A = \{b_1, b_2, b_3, b_4\}, \quad F_B = \{b_4, b_5, b_6, b_7\}, \quad F_C = \{b_7, b_8, b_{11}, b_{10}\}, \\ F_D = \{b_{10}, b_9, b_8, b_6\}, F_{OH-3} = \{b_{17}\}, \quad F_{OH-17} = \{b_{18}, b_{19}\}.$$

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

$$M_{\text{rings}} = \{F_A, F_B, F_C, F_D\}, \\ M_{\text{hydroxyl}} = \{F_{OH-3}, F_{OH-17}\}.$$

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

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

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 $0 \leq k \leq n$, define the k -flattening map*

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

applied recursively k times. Then

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

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. \square

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. \square

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. \square

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 . \square

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 $v \in V_H$,*

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

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 $\varphi_k: \mathcal{P}^n(V_0) \rightarrow \mathcal{P}^{n-k}(V_0)$ 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 . \square

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 $v \in V_H$,*

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

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. \square

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. \square

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 [103, 104], Intuitionistic Fuzzy Sets [5, 6], Vague Sets [3, 39], Rough Sets [69, 70], Bipolar Fuzzy Sets [2], HyperFuzzy Sets [22, 50, 84], Picture Fuzzy Sets [14, 46], Hesitant Fuzzy Sets [86, 87], and Neutrosophic Sets [78, 83].

We also plan to investigate their more recent extensions, such as Quadripartitioned Neutrosophic Sets [36, 55, 100], Plithogenic Sets [27, 33, 34], and HyperPlithogenic Sets [28–30]. 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.

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

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

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