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Fuzzy Order-Theoretic Models for Molecular Structures Based on Property-Induced Posets with Connections to Baer Semigroups

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Abstract

In chemical systems, molecular properties such as electronegativity are often subject to uncertainty due to environmental fluctuations, measurement errors, or intrinsic variability. Fuzzy set theory provides a framework to model such uncertainties, allowing chemical descriptors to be expressed as degrees of membership rather than fixed values. This paper develops a rigorous order-theoretic framework for studying fuzzy structures arising from property-induced partially ordered sets (posets) in molecular systems. By extending classical poset theory through fuzzy relations, we formalize graded comparability and inclusion principles that naturally occur in chemical and molecular structures. The proposed approach preserves essential order-theoretic properties while allowing flexible representation of uncertainty.

We further establish a connection between fuzzy molecular relations and abstract algebra by mapping these relations onto Baer $*$-semigroups, algebraic structures with zero elements and idempotent-generated annihilators. We present a structure theorem for finite

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Baer $*$-semigroups, develop an $O(n^3)$ recognition algorithm, and prove categorical completeness and cocompleteness. Applications to functional group classification, reaction mechanism modeling, stereochemistry, pharmacophore analysis, and QSAR enhancement demonstrate the practical utility of the framework. Illustrative examples show that the fuzzy poset approach captures resonance effects and stereochemical hierarchies, providing a unified mathematical tool for chemical informatics that bridges computational chemistry and abstract algebra.

1 Introduction

1.1 Background and motivation

The study of chemical systems often involves quantifying molecular properties such as electronegativity, polarity, and hydrogen bonding potential. Chemical graph theory provides a natural representation of molecular structures as vertices and edges [1,16], with topological indices and molecular descriptors characterizing molecular similarity and reactivity [11,14]. Traditionally, these properties are treated as fixed numerical descriptors; however, environmental fluctuations, measurement imprecision, and intrinsic variability introduce uncertainty in chemical systems [19,21].

Fuzzy set theory, pioneered by Zadeh [19], provides a natural framework to model these uncertainties, allowing molecular properties to be expressed as degrees of membership rather than exact values [10,20]. Such fuzzy molecular descriptors facilitate robust similarity analysis, reaction prediction, and pharmacophore modeling in computational chemistry.

Order theory provides a fundamental mathematical framework for modeling hierarchical and relational structures [6]. Property-induced posets arise when elements are compared based on chemical or structural attributes [3,11]. Electronegativity, a measure of an atom's ability to attract electrons, plays a central role in determining molecular reactivity and interaction patterns, building upon foundational concepts established by Pauling [12]. Extending these constructions to a fuzzy framework allows modeling of partial dominance, approximate ordering, and graded comparability [17,20].

Chemical intuition often involves hierarchical reasoning: oxygen is "more electronegative" than carbon, double bonds are "stronger" than single bonds, and chiral centers have "priority" rankings according to established rules like the Cahn-Ingold-Prelog system [4]. These intuitive hierarchies, when formalized mathematically as partial orders, enable several significant applications:

(a) Systematic functional group classification

(b) Quantitative reaction mechanism analysis

(c) Stereochemical characterization

(d) Pharmacophore modeling

(e) Property prediction in drug design

Parallel to these developments, abstract algebra—particularly semigroup theory—offers tools to study structures defined by annihilator properties. Baer semigroups, introduced by Foulis [7, 8], are semigroups with zero in which every left and right annihilator is generated by an idempotent. Such semigroups appear naturally in multiplicative semigroups of Baer rings [2], transformation semigroups [15], and operator algebras. Recent advances in fuzzy mathematical methods [18] provide additional context for integrating these frameworks with computational chemistry.

1.2 Research objectives and contributions

The primary objectives of this research are:

1. Establish a rigorous mathematical foundation for property-induced partial orders in molecular systems
2. Develop formal methods for analyzing molecular structure and reactivity using order theory
3. Extend the framework to fuzzy settings for handling chemical uncertainty
4. Demonstrate practical applications in key areas of organic chemistry

5. Establish connections between fuzzy molecular descriptors and abstract algebraic structures (Baer semigroups)

This paper makes the following specific contributions:

1. Formal construction of property-induced posets with well-definedness proofs (Theorems 3.1, 3.3, 3.5)
2. Structure theorems for molecular posets (Theorems 3.2, 3.6)
3. Functional group classification scheme based on poset isomorphism
4. Reaction analysis framework as poset trajectories (Theorem 5.1)
5. Stereochemical formalization connecting CIP rules to order theory (Theorem 6.2)
6. Fuzzy extensions with Type-2 fuzzy partial orders (Theorems 10.1, 10.5)
7. Structure theorems for finite Baer $*$-semigroups and $O(n^3)$ recognition algorithm
8. Categorical completeness results for Baer semigroups
9. Pharmaceutical applications to pharmacophore modeling and QSAR enhancement

1.3 Organization of the paper

The remainder of this paper is organized as follows: Section 2 reviews the necessary mathematical background in order theory, fuzzy mathematics, and semigroup theory. Section 3 formally constructs property-induced partial orders and establishes their fundamental properties. Section 4 applies poset theory to functional group classification. Section 5 analyzes chemical reaction mechanisms. Section 6 formalizes stereochemical concepts. Section 7 introduces Baer semigroups and establishes their fundamental properties. Section 8 presents the structure and classification of finite Baer semigroups. Section 9 extends the framework to fuzzy settings and connects to Baer structures. Section 10 demonstrates pharmaceutical applications. Section 11 discusses computational implementation. Section 12 presents categorical aspects. Section 13 concludes with a summary of contributions and future research directions.

2 Mathematical foundations

2.1 Order-theoretic preliminaries

Definition 2.1 (Partially Ordered Set). A *partially ordered set (poset)* $(P, \leq)$ consists of a set P with a binary relation $\leq$ satisfying:

1. **Reflexivity:** $\forall x \in P,\ x \leq x$
2. **Antisymmetry:** $\forall x, y \in P,\ (x \leq y \wedge y \leq x) \Rightarrow x = y$
3. **Transitivity:** $\forall x, y, z \in P,\ (x \leq y \wedge y \leq z) \Rightarrow x \leq z$

Definition 2.2 (Hasse Diagram). For a finite poset $(P, \leq)$, the *Hasse diagram* is a directed graph where:

- Elements of P are represented as vertices
- An edge is drawn upward from x to y if $x < y$ (i.e., $x \leq y$ and $x \neq y$)
- Edges are drawn only for *cover relations*: $x < y$ and $\nexists z$ such that $x < z < y$

Definition 2.3 (Chain and Antichain). Let $(P, \leq)$ be a poset. A subset $C \subseteq P$ is a *chain* if for all $x, y \in C$, either $x \leq y$ or $y \leq x$. A subset $A \subseteq P$ is an *antichain* if for all distinct $x, y \in A$, neither $x \leq y$ nor $y \leq x$ holds.

Definition 2.4 (Order Embedding). A map $\phi : (P, \leq_P) \to (Q, \leq_Q)$ between posets is an *order embedding* if for all $x, y \in P$:

$$x \leq_P y \iff \phi(x) \leq_Q \phi(y)$$

Theorem 2.1 (Dilworth's Theorem). *In any finite poset, the minimum number of chains needed to partition the set equals the size of a maximum antichain.*

Theorem 2.2 (Mirsky's Theorem)**.** *In any finite poset, the minimum number of antichains needed to partition the set equals the length of a maximum chain.*

2.2 Fuzzy set theory basics

Definition 2.5 (Fuzzy Set)**.** Let X be a universe of discourse. A *fuzzy set* A in X is characterized by a membership function $\mu_A : X \to [0, 1]$, where $\mu_A(x)$ represents the degree of membership of x in A.

Definition 2.6 (Fuzzy Relation)**.** A *fuzzy binary relation* R on X is a fuzzy subset of $X \times X$ with membership function $\mu_R : X \times X \to [0, 1]$.

Definition 2.7 (Fuzzy Partial Order)**.** A *fuzzy partial order* on a set X is a fuzzy relation $\mu : X \times X \to [0, 1]$ satisfying for all $x, y, z \in X$:

1. $\mu(x, x) = 1$ (fuzzy reflexivity)
2. If $\mu(x, y) > 0$ and $\mu(y, x) > 0$, then $x = y$ (fuzzy antisymmetry)
3. $\mu(x, z) \geq \sup_{y \in X} \min\{\mu(x, y), \mu(y, z)\}$ (fuzzy transitivity)

The pair (X, μ) is called a *fuzzy poset.*

Definition 2.8 (α-cut)**.** For a fuzzy relation μ and $\alpha \in [0, 1]$, the α-cut is the crisp relation:

$$R_\alpha = \{(x, y) \in X \times X \mid \mu(x, y) \geq \alpha\}$$

Proposition 2.3. *If (X, μ) is a fuzzy poset, then for each $\alpha \in (0, 1]$, the α-cut R_α is a crisp partial order on X.*

2.3 Semigroup theory preliminaries

Definition 2.9. A **semigroup** is a set S equipped with an associative binary operation $\cdot : S \times S \to S$. An element $0 \in S$ is a **zero** if $0x = x0 = 0$ for all $x \in S$. An element $1 \in S$ is an **identity** if $1x = x1 = x$ for all $x \in S$.

Definition 2.10. For a semigroup S with zero and any subset $X \subseteq S$, define:

- **Left annihilator**: $\mathrm{L}(X) = \{s \in S \mid sx = 0 \text{ for all } x \in X\}$
- **Right annihilator**: $\mathrm{R}(X) = \{s \in S \mid xs = 0 \text{ for all } x \in X\}$

For a singleton set $X = \{a\}$, we write $\mathrm{L}(a)$ and $\mathrm{R}(a)$.

Definition 2.11. An element $e \in S$ is **idempotent** if $e^2 = e$. The set of idempotents is denoted $E(S)$.

Definition 2.12 (Green's Relations)**.** For $a, b \in S$:

- $a\mathcal{L}b$ iff $S^1a = S^1b$ (where S^1 is S with identity adjoined)
- $a\mathcal{R}b$ iff $aS^1 = bS^1$
- $a\mathcal{H}b$ iff $a\mathcal{L}b$ and $a\mathcal{R}b$
- $a\mathcal{D}b$ iff $\exists c \in S : a\mathcal{L}c$ and $c\mathcal{R}b$

An $\mathcal{H}$-class containing an idempotent is a maximal subgroup of S.

Definition 2.13. A semigroup S is **regular** if for every $a \in S$, there exists $b \in S$ such that $aba = a$.

Definition 2.14. A semigroup S is **inverse** if for every $a \in S$, there exists a unique $a^{-1} \in S$ such that $aa^{-1}a = a$ and $a^{-1}aa^{-1} = a^{-1}$.

2.4 Chemical property functions

Definition 2.15 (Chemical Property Function)**.** A *chemical property function* for a molecule M with component set C (atoms or bonds) is a function $f : C \to \mathbb{R}$ assigning a quantitative value to each component.

Common chemical property functions include:

- Electronegativity: $\chi : V \to \mathbb{R}$ (Pauling scale)
- Valence: $v : V \to \mathbb{N}$ (number of bonds)
- Bond energy: $\mathrm{BE} : E \to \mathbb{R}^+$ (dissociation energy)

- Atomic radius: $r : V \to \mathbb{R}^+$
- Polarizability: $\alpha : V \to \mathbb{R}^+$

Table 1. Pauling electronegativity values for common elements

Element	Electronegativity (χ)
H	2.20
C	2.55
N	3.04
O	3.44
F	3.98
Cl	3.16
Br	2.96
I	2.66
S	2.58
P	2.19

3 Property-induced partial orders

Remark. All property-induced orders are considered on equivalence classes of chemically indistinguishable atoms or bonds, ensuring antisymmetry. Specifically, we work on the quotient set $V/\sim$ where $a \sim b$ iff $\chi(a) = \chi(b)$ (or the analogous equivalence for other properties).

3.1 Electronegativity-induced posets

Definition 3.1 (Electronegativity Poset)**.** Let M be a molecule with atom set V. Define the *electronegativity poset* $(V, \leq_\chi)$ by:

$$a \leq_\chi b \iff \chi(a) \leq \chi(b)$$

where $\chi : V \to \mathbb{R}$ is the Pauling electronegativity function.

Theorem 3.1. *For any molecule M, after quotienting by chemical equivalence (i.e., identifying atoms with identical electronegativity), $(V, \leq_\chi)$ is a partially ordered set.*

Proof. Reflexivity: $\chi(a) \leq \chi(a)$ always holds, so $a \leq_\chi a$.

Antisymmetry: If $a \leq_\chi b$ and $b \leq_\chi a$, then $\chi(a) \leq \chi(b)$ and $\chi(b) \leq \chi(a)$, hence $\chi(a) = \chi(b)$. By construction we identify such atoms, so $a = b$ in the quotient.

Transitivity: If $a \leq_\chi b$ and $b \leq_\chi c$, then $\chi(a) \leq \chi(b) \leq \chi(c)$, so $\chi(a) \leq \chi(c)$ and thus $a \leq_\chi c$. ■

Example 3.1 (Water Molecule)**.** For water (H_2O), $\chi(\mathrm{O}) = 3.44$, $\chi(\mathrm{H}) = 2.20$. The electronegativity poset has:

$$\mathrm{H} <_\chi \mathrm{O}, \quad \mathrm{H} <_\chi \mathrm{O}$$

with the two hydrogen atoms forming an antichain at the bottom level.

Water Electronegativity Poset

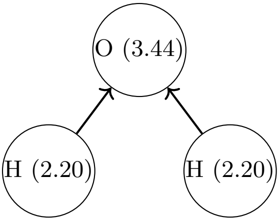


Figure 1. Hasse diagram of the electronegativity poset for water

Theorem 3.2 (Structure Theorem)**.** *Let M be a molecule with n distinct atom types $A_1, \ldots, A_n$ ordered by increasing electronegativity: $\chi(A_1) < \chi(A_2) < \cdots < \chi(A_n)$. Then the Hasse diagram of $(V, \leq_\chi)$ has exactly n levels, with level i containing all atoms of type A_i.*

Proof. For each atom $a \in V$, there exists exactly one i such that a is of type A_i. By definition of $\leq_\chi$, all atoms of type A_i are mutually incomparable (equal electronegativity), and for any $i < j$, every atom of type A_i is less than every atom of type A_j. Thus the Hasse diagram has n levels with level i corresponding to atom type A_i. ■

Example 3.2 (Ethanol)**.** Ethanol (C_2H_5OH) contains atoms: 2 C ($\chi = 2.55$), 6 H ($\chi = 2.20$), 1 O ($\chi = 3.44$). The electronegativity poset has three levels:

- Level 1: 6 H atoms (antichain)
- Level 2: 2 C atoms (antichain)
- Level 3: 1 O atom

All H atoms are below all C atoms, which are below the O atom.

3.2 Valence-induced posets

Definition 3.2 (Valence Poset)**.** For a molecule M with atom set V, define the *valence poset* $(V, \leq_v)$ by:

$$a \leq_v b \iff v(a) \leq v(b)$$

where $v(a)$ denotes the number of bonds atom a forms in M.

Theorem 3.3. *For any molecule M, $(V, \leq_v)$ is a poset after quotienting by chemical equivalence.*

Proof. Analogous to Theorem 3.1, using the fact that valence is a function $V \to \mathbb{N}$ and $\leq$ on $\mathbb{N}$ is a total order. ■

Theorem 3.4 (Hydrocarbon Poset Coincidence)**.** *For any hydrocarbon molecule consisting solely of carbon and hydrogen atoms, the valence poset and the electronegativity poset are isomorphic. In both posets, every hydrogen atom is strictly below every carbon atom, and atoms of the same element are incomparable (forming antichains). Consequently, the Hasse diagram has exactly two levels: the lower level contains all hydrogen atoms, and the upper level contains all carbon atoms.*

Proof. In a hydrocarbon, each hydrogen atom forms exactly one bond, so its valence is $v(\mathrm{H}) = 1$; each carbon atom forms four bonds, so $v(\mathrm{C}) = 4$. Thus for any hydrogen atom H and any carbon atom C, we have $v(H) < v(C)$, which gives $H <_v C$ in the valence poset.

Similarly, the Pauling electronegativity of hydrogen is approximately 2.20 and that of carbon is approximately 2.55; hence $\chi(H) < \chi(C)$ and therefore $H <_\chi C$ in the electronegativity poset.

All hydrogen atoms have identical valence and electronegativity, so they are pairwise incomparable in both posets; likewise, all carbon atoms are pairwise incomparable. Hence the two posets have the same comparability structure (a two-level poset with a lower antichain of hydrogens and an upper antichain of carbons) and are therefore isomorphic. ■

Remark. This coincidence is specific to hydrocarbons and does not hold for heteroatomic molecules (e.g., alcohols or amines) where electronegativity and valence orders differ.

3.3 Bond energy posets

Definition 3.3 (Bond Energy Poset)**.** For a molecule M with bond set E, define the *bond energy poset* $(E, \leq_{\mathrm{BE}})$ by:

$$e_1 \leq_{\mathrm{BE}} e_2 \iff \mathrm{BE}(e_1) \leq \mathrm{BE}(e_2)$$

where $\mathrm{BE} : E \to \mathbb{R}^+$ gives the bond dissociation energy.

Theorem 3.5. *For any molecule M, $(E, \leq_{BE})$ is a poset after quotienting by chemical equivalence.*

Proof. Analogous to Theorem 3.1, using bond energies instead of electronegativities. ■

Theorem 3.6 (Symmetry Detection)**.** *A molecule M has symmetric bonds if and only if its bond energy poset $(E/\sim, \leq_{BE})$ contains an antichain of size greater than one after quotienting by bond–energy equivalence.*

Proof. ($\Rightarrow$) If two bonds e_1 and e_2 are chemically symmetric then $\mathrm{BE}(e_1) = \mathrm{BE}(e_2)$. They belong to the same equivalence class and form an antichain of size greater than one in the quotient poset.

($\Leftarrow$) If the quotient poset contains an antichain with more than one element, then those bonds have equal bond energy and correspond to symmetric bond environments. ■

Table 2. Typical bond dissociation energies (kJ/mol)

Bond	Energy (kJ/mol)
C-C	348
C=C	614
C≡C	839
C-H	413
C-O	360
C=O	799
O-H	463
N-H	391

Example 3.3 (Benzene)**.** Benzene (C_6H_6) has six carbon-carbon bonds. In the resonance hybrid, all C-C bonds have equal bond order (1.5) and approximately equal bond energies. Therefore, in the bond energy poset, all six C-C bonds form an antichain of size 6, reflecting the hexagonal symmetry of the molecule.

3.4 Combined property posets

Definition 3.4 (Lexicographic Product Poset)**.** Given chemical property functions $f_1, \ldots, f_k$ with associated posets $(C, \leq_{f_1}), \ldots, (C, \leq_{f_k})$, define the *lexicographic product poset* $(C, \leq_{\text{lex}})$ by:

$$x \leq_{\text{lex}} y \iff \exists i \in \{1, \ldots, k\} \text{ such that } f_j(x) = f_j(y) \text{ for } j < i \text{ and } f_i(x) < f_i(y)$$

Theorem 3.7. *For any set of chemical property functions, the lexicographic product poset is a well-defined poset after quotienting by chemical equivalence.*

Proof. Let C be the set of molecular components (atoms or bonds). For each $x \in C$ form the tuple $(f_1(x), \ldots, f_k(x))$. The lexicographic order $\leq_{\text{lex}}$ on $\mathbb{R}^k$ is a partial order (in fact a total order). Define a relation $\preceq$ on C by

$$x \preceq y \iff (f_1(x), \ldots, f_k(x)) \leq_{\text{lex}} (f_1(y), \ldots, f_k(y)).$$

Reflexivity and transitivity follow directly from the corresponding properties of $\leq_{\text{lex}}$. For antisymmetry, if $x \preceq y$ and $y \preceq x$, then the two tuples are equal, so $f_i(x) = f_i(y)$ for all i. After quotienting C by the equivalence relation

$$x \sim y \iff f_i(x) = f_i(y) \text{ for all } i,$$

the induced order on the quotient set becomes a partial order. ■

Example 3.4 (Amino Acids)**.** For amino acids, one might consider lexicographic order based on (hydrophobicity, charge, size) to classify residues for protein structure prediction.

4 Functional group classification

4.1 Poset isomorphism of functional groups

Definition 4.1 (Poset Isomorphism)**.** Two molecules M_1 and M_2 are *poset-isomorphic* if their electronegativity posets $(V_1, \leq_{\chi_1})$ and $(V_2, \leq_{\chi_2})$ are isomorphic as posets.

Definition 4.2 (Labeled Poset)**.** A *labeled poset* is a poset $(P, \leq)$ together with a labeling function $\ell : P \to L$ assigning a label (element type) to each element.

Remark (Classification of Functional Groups by Electronegativity Posets)*.* The electronegativity posets of common organic functional groups fall into a few isomorphism classes when considered as unlabeled posets. For example:

- **Two-element chains:** carbonyl (C=O), hydroxyl (OH), thiol (SH), etc.
- **V-shaped posets** (one element above two incomparable ones): amine (NH_2), nitro (NO_2).
- **Three-level posets**: carboxyl (COOH), phosphate (PO_4H_2), etc.

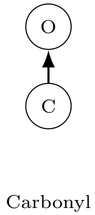
When each atom is labeled by its chemical identity (e.g., C, H, O, N), the resulting *labeled* poset uniquely determines the functional group up to symmetry. For instance:

- Carbonyl (C=O): atoms C ($\chi \approx 2.55$) and O ($\chi \approx 3.44$) give a two-element chain $C < O$.
- Hydroxyl (OH): atoms H ($\chi \approx 2.20$) and O give $H < O$, also a two-element chain.
- Amine (NH_2): atoms N ($\chi \approx 3.04$) and two H atoms produce a V-shape: the two H's are incomparable and both are below N.
- Nitro (NO_2): atoms N and two O atoms give a V-shape but with the O's above N (since $\chi(\mathrm{O}) > \chi(\mathrm{N})$).
- Carboxyl (COOH): atoms C, two O atoms, and one H. Typical electronegativities yield a three-level structure: H at the bottom, C in the middle, and the two O's at the top (both above C, incomparable with each other).

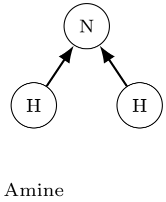
As unlabeled posets, carbonyl and hydroxyl are isomorphic (both are two-element chains), amine and nitro are isomorphic (both are V-shaped), etc. However, once we attach the atom labels, the structures become distinct because the labels differ. Hence the labeled electronegativity poset, together with the molecular bonding graph, provides a complete invariant that characterizes each functional group uniquely (up to graph isomorphism).

Table 3. Poset classification of common functional groups

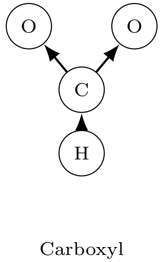
Functional Group	Formula	Atom Set	Poset Type	Hasse Diagram
Carbonyl	C=O	{C,O}	2-element chain	C < O
Hydroxyl	OH	{H,O}	2-element chain	H < O
Amine	NH_2	{N,H,H}	V-shape	H,H < N
Nitro	NO_2	{N,O,O}	V-shape (inverted)	N < O,O
Carboxyl	COOH	{C,O,O,H}	3-level	H < C < O,O
Methyl	CH_3	{C,H,H,H}	2-level	H,H,H < C
Sulfhydryl	SH	{S,H}	2-element chain	H < S
Aldehyde	CHO	{C,H,O}	2-level with chain	H,C < O
Ether	C-O-C	{C,O,C}	2-level	C,C < O



(a) Two-element chain



(b) V-shape



(c) Three-level

Figure 2. Hasse diagrams of functional group posets

4.2 Algorithm for functional group identification

Algorithm 1 Functional Group Recognition

```
Input: Molecular structure $M$
Extract atom set $V$ and compute electronegativity values $\chi(v)$ for all $v \in V$
Construct electronegativity poset $(V, \leq_\chi)$
Compute poset invariants: size, height, width, number of levels
Identify connected components of the poset (corresponding to separate functional groups)
for each connected component $P_i$ do
    Compute the labeled Hasse diagram with atom type labels
    Compare with database of functional group poset templates
    Record matching functional group with confidence score
end for
Output: Identified functional groups with confidence scores
```

4.3 Isomorphism and automorphism groups

Definition 4.3 (Automorphism Group)**.** For a molecular poset $(V, \leq_\chi)$, the *automorphism group* $\mathrm{Aut}(V, \leq_\chi)$ consists of all bijections $\phi : V \to V$ that preserve the order: $x \leq_\chi y \iff \phi(x) \leq_\chi \phi(y)$.

Theorem 4.1. *If atoms are distinguished only by their electronegativity values (ignoring bonding constraints), then the automorphism group of the electronegativity poset is the direct product of symmetric groups acting on the sets of atoms having equal electronegativity:*

$$\mathrm{Aut}(V, \leq_\chi) \cong S_{n_1} \times S_{n_2} \times \cdots \times S_{n_k}$$

where n_i is the number of atoms of type A_i (all with equal electronegativity) and k is the number of distinct atom types.

Proof. In the electronegativity poset, atoms of the same type form an antichain and are mutually incomparable. Atoms of different types are totally ordered by electronegativity. Any automorphism must preserve the order, hence must map atoms to atoms of the same type (since types are distinguished by their position in the order). Within each type, any permutation preserves the order because all atoms of that type are incomparable. Thus the automorphism group is the direct product of the full symmetric groups on each type. ■

Remark. This theorem describes the automorphism group of the abstract poset; actual molecular automorphisms must also preserve bonding, which may impose additional restrictions.

Example 4.1 (Water Automorphism)**.** For water (H_2O), we have two H atoms (type A_1) and one O atom (type A_2). The automorphism group is $S_2 \times S_1 \cong S_2$, which exchanges the two hydrogen atoms while fixing the oxygen atom. This corresponds to the molecular symmetry of water.

5 Reaction mechanism analysis

5.1 Reaction poset trajectories

Definition 5.1 (Reaction Poset Trajectory)**.** For a chemical reaction $R : A \to B$, a *reaction poset trajectory* is a sequence of posets $(P_0, P_1, \ldots, P_n)$ where:

- P_0 is the electronegativity poset of reactant A;
- P_n is the electronegativity poset of product B;
- Each P_i represents an intermediate state (transition state or resonance hybrid).

All posets are taken after quotienting by chemical equivalence.

Definition 5.2 (Poset Morphism)**.** A *poset morphism* $f : (P, \leq_P) \to (Q, \leq_Q)$ is an order-preserving map: if $x \leq_P y$ then $f(x) \leq_Q f(y)$.

Definition 5.3 (Reaction Pathway)**.** A *reaction pathway* is a sequence of poset morphisms:

$$P_0 \xrightarrow{f_1} P_1 \xrightarrow{f_2} \cdots \xrightarrow{f_n} P_n$$

where each f_i represents the electronic reorganization step.

5.2 SN2 reaction evolution

Theorem 5.1 (SN2 Reaction Evolution)**.** *For the bimolecular nucleophilic substitution (SN2) reaction*

$$\mathrm{CH_3Cl + OH^-} \;\longrightarrow\; \mathrm{CH_3OH + Cl^-},$$

the electronegativity poset passes through three non-isomorphic posets along the reaction coordinate.

Proof. We use the Pauling electronegativity values (rounded to two decimals):

$$\chi(\mathrm{H}) = 2.20, \quad \chi(\mathrm{C}) = 2.55, \quad \chi(\mathrm{Cl}) = 3.16, \quad \chi(\mathrm{O}) = 3.44.$$

Stage 1 (Reactants). The reactants are separate species:

- $\mathrm{CH_3Cl}$ contains atoms $\{C,\ 3H,\ Cl\}$. Their electronegativities give the strict order $H < C < Cl$, and the three hydrogen atoms are mutually incomparable (an antichain of size 3). Hence the Hasse diagram of this component is a three-level poset with a three-element antichain at the bottom.
- $\mathrm{OH^-}$ contains $\{O,\ H\}$ with $H < O$, a two-element chain.

The two species are not covalently linked, so the overall poset P_0 is the disjoint union of these two components. Consequently P_0 has two connected components, heights 3 and 2.

Stage 2 (Transition State). In the transition state $[\mathrm{HO \cdots CH_3 \cdots Cl}]^\ddagger$ all atoms are bound in a single hypervalent assembly. The atom set is $\{O,\ Cl,\ C,\ 4H\}$ (the three methyl H's plus the hydroxide H). The electronegativity order is

$$H < C < Cl < O,$$

with all four hydrogen atoms having identical χ and therefore forming an antichain of size 4 at the bottom. Thus P_1 is a single connected poset whose Hasse diagram consists of a four-level chain $H < C < Cl < O$

where the bottom level contains four incomparable elements. Its height is 4, width 4, and it is connected.

Stage 3 (Products). The products are separate:

- CH_3OH contains $\{C,\ O,\ 4H\}$ (three methyl H's and one hydroxyl H). All hydrogen atoms have equal electronegativity, so they form an antichain of size 4. The order is $H < C < O$ because $\chi(H) < \chi(C) < \chi(O)$. Hence this component is a connected three-level poset with a four-element antichain at the bottom.
- Cl^- is a single ion, represented by a one-element poset (a singleton, height 1).

The overall poset P_2 is the disjoint union of these two components. It has two connected components, heights 3 and 1.

Non-isomorphism. The three posets are pairwise non-isomorphic:

- P_0 has two components, heights 3 and 2; P_1 is connected (one component) of height 4; P_2 has two components, heights 3 and 1.
- The maximal antichain sizes differ: P_0 has a maximal antichain of size 3; P_1 has size 4; P_2 has size 4 but its components are of different heights.

Therefore the electronegativity poset evolves through three non-isomorphic posets. ■

5.3 Energy landscape and poset invariants

Definition 5.4 (Poset Energy)**.** For a reaction trajectory $(P_0, P_1, \ldots, P_n)$, define the *poset energy* of P_i as

$$E(P_i) = \sum_{a \lessdot b} \bigl|\chi(b) - \chi(a)\bigr|,$$

where $a \lessdot b$ denotes a cover relation in the Hasse diagram of P_i. (If P_i is disconnected, the sum is taken over all cover relations of all components.)

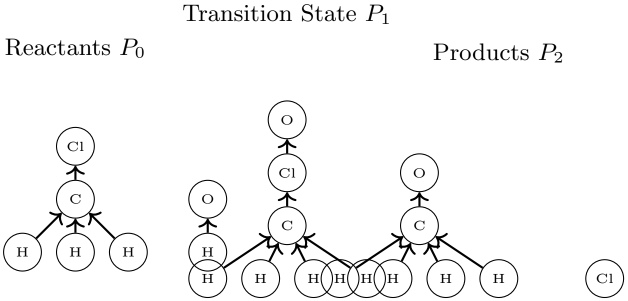


Figure 3. Electronegativity poset evolution in SN2 reaction

Cover relations represent the strongest electronegativity hierarchies between directly interacting atoms; therefore the sum of electronegativity differences along cover relations measures the degree of bond polarization within the molecular structure.

Definition 5.5 (Poset Reactivity Index)**.** For a molecule M, define the *poset reactivity index* as:

$$R(M) = \frac{\text{height}(P) \times \text{width}(P)}{|V|}$$

where P is the electronegativity poset.

Conjecture 5.1 (Energy Barrier Correspondence)**.** *For the SN2 reaction studied above, the poset energy $E(P_i)$ attains its maximum at the transition state (P_1), reflecting the high degree of bond polarization and partial charge separation.*

5.4 Electrophilic aromatic substitution

Example 5.1 (Nitration of Benzene)**.** In electrophilic aromatic substitution, benzene undergoes nitration to form nitrobenzene. The reaction trajectory involves:

1. Benzene: All C atoms have equal electronegativity, forming an an-

tichain of size 6 at one level, with H atoms below.

2. σ-complex (Wheland intermediate): One carbon becomes sp^3 hybridized, breaking aromaticity. Its electronegativity changes, creating a hierarchical structure.
3. Nitrobenzene: Returns to aromatic system but with NO_2 group attached, creating a V-shaped poset for the nitro group.

The poset trajectory reflects the temporary loss and restoration of symmetry.

6 Stereochemistry and chirality

6.1 CIP posets

Definition 6.1 (CIP Poset)**.** For a chiral center with substituents a, b, c, d, define the *Cahn-Ingold-Prelog poset* $(S, \leq_{CIP})$ where $S = \{a, b, c, d\}$ and $x \leq_{CIP} y$ if substituent x has lower CIP priority than y.

Theorem 6.1 (CIP Priority Rules as Total Order)**.** *The Cahn-Ingold-Prelog priority rules define a total order on the set of substituents attached to a chiral center.*

Proof. The CIP rules provide a deterministic comparison procedure for any pair of substituents. The first criterion compares the atomic numbers of the atoms directly bonded to the stereocenter; higher atomic number gives higher priority. If these are equal, the comparison proceeds to the next atoms along the substituent chains, considering atomic numbers lexicographically. Isotopic mass is used when atomic numbers coincide. This procedure is:

- Reflexive: A substituent has the same priority as itself.
- Antisymmetric: If x has higher priority than y and y has higher priority than x, then x and y are identical substituents.
- Transitive: Priority comparisons are consistent.

- Total: Any two distinct substituents can be compared.

Thus the priority relation is a total order, which is a special case of a partially ordered set. ■

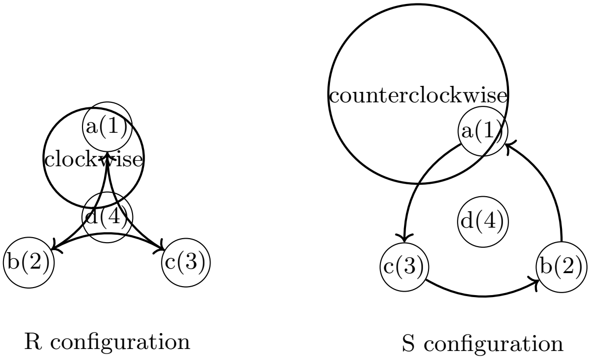
Theorem 6.2 (Enantiomeric Duality)**.** *For a chiral molecule with substituents a, b, c, d where $a <_{CIP} b <_{CIP} c <_{CIP} d$, the two enantiomers correspond to opposite orientations of the same totally ordered CIP poset embedded in three-dimensional space.*

Proof. Let $P = (\{a, b, c, d\}, \leq_{CIP})$ with $a < b < c < d$ (total order by priority).

The R configuration corresponds to clockwise arrangement when the lowest priority substituent (d) is oriented away, typically yielding order $a \to b \to c$.

The S configuration corresponds to counterclockwise arrangement $a \to c \to b$.

Both are geometric realizations of P preserving $a < b$, $a < c$, $a < d$, $b < d$, $c < d$, differing only in the spatial arrangement of b and c. ■



(a) R configuration **(b)** S configuration

Figure 4. Enantiomeric orientations of CIP poset

6.2 Meso compounds and symmetry

Definition 6.2 (Molecular Poset with Stereochemistry)**.** A *molecular poset with stereochemistry* is a labeled poset $(V, \leq, \sigma)$ where $\sigma : V \to \{R, S, \text{achiral}\}$ assigns stereochemical configuration to each stereogenic center.

Theorem 6.3 (Meso Compound Criterion)**.** *Let M be a molecule with at least two stereogenic (chiral) centers and let $(P, \leq, \sigma)$ be its labeled molecular poset with stereochemistry. Then M is a meso compound (i.e., achiral despite containing chiral centers) if and only if the labeled poset admits a non-trivial automorphism $\phi : P \to P$ of order two that exchanges the corresponding stereogenic centers while preserving adjacency and labels but inverting configuration ($\sigma(\phi(x))$ = opposite of $\sigma(x)$ for stereogenic centers).*

Proof. ($\Rightarrow$) Assume M is a meso compound. By definition, a meso compound possesses an internal symmetry (typically a mirror plane or inversion center) that maps the molecule onto itself while reversing the configurations of the stereogenic centers.

This geometric symmetry induces a bijection $\phi : P \to P$ on the elements of the molecular poset. Because chemical bonds and structural relationships are preserved under the symmetry, the partial order relation is preserved; that is, $x \leq y \iff \phi(x) \leq \phi(y)$. Thus ϕ is a poset automorphism.

For stereogenic centers, the symmetry maps each center to its mirror-image counterpart, so $\sigma(\phi(x))$ is the opposite configuration of $\sigma(x)$. Applying the symmetry twice restores the original configuration, so $\phi^2 = \text{id}$. Since ϕ is not the identity (it exchanges centers), it is a non-trivial automorphism of order two.

($\Leftarrow$) Conversely, suppose the labeled poset $(P, \leq, \sigma)$ admits a non-trivial automorphism ϕ with $\phi^2 = \text{id}$ that exchanges stereogenic centers while preserving bonding relations and inverting configurations.

Because ϕ preserves adjacency and the structural ordering of atoms, it corresponds to a symmetry of the molecular graph. The fact that ϕ has order two means that applying the transformation twice returns every atom to its original position. Such a transformation represents a reflection or inversion symmetry of the molecule.

This symmetry maps each stereogenic center to its mirror-related counterpart with opposite configuration, making the molecule superimposable on its mirror image. Hence the molecule is achiral despite containing stereogenic centers, and therefore it is a meso compound. ■

Example 6.1 (Tartaric Acid)**.** Tartaric acid (HOOC-CH(OH)-CH(OH)-COOH) has two stereogenic centers. The meso form has an internal symmetry plane that exchanges the two centers while inverting their configurations. The labeled poset has an automorphism swapping the two CH(OH) groups.

6.3 Diastereomer classification

Definition 6.3 (Diastereomeric Posets)**.** Two diastereomers are *poset-distinct* if their molecular posets (with stereochemistry) are non-isomorphic as labeled posets.

Theorem 6.4 (Diastereomer Discrimination)**.** *Diastereomers have non-isomorphic labeled posets because the relative ordering of substituents differs between them.*

Example 6.2 (Threonine Diastereomers)**.** Threonine (CH_3-CH(OH)-CH(NH_2)-COOH) has two stereogenic centers. The four stereoisomers are:

- (2S,3S)-threonine
- (2R,3R)-threonine (enantiomer of above)
- (2S,3R)-allo-threonine
- (2R,3S)-allo-threonine (enantiomer of above)

The threonine and allo-threonine diastereomers have different spatial arrangements of substituents around the two centers, leading to non-isomorphic labeled posets when stereochemical configuration is included.

7 Baer semigroups: definitions and basic properties

The algebraic structures arising from molecular posets naturally lead to semigroup-like composition laws when considering successive reaction transformations. In particular, annihilator conditions in semigroup theory provide a useful algebraic framework for describing reaction constraints and forbidden pathways. In reaction systems, certain combinations of molecular transformations are forbidden because they annihilate reactive intermediates. These annihilator conditions naturally lead to Baer semigroup structures in which reaction steps compose while preserving annihilator constraints. This motivates the introduction of Baer semigroups and Baer $*$-semigroups, which capture annihilator-based structures analogous to those encountered in chemical systems.

7.1 Definition and first properties

Definition 7.1. A semigroup S with zero element 0 is called a **Baer semigroup** if for every $x \in S$:

1. $\mathrm{L}(x) = Se$ for some idempotent $e \in S$;
2. $\mathrm{R}(x) = fS$ for some idempotent $f \in S$.

That is, every left annihilator is a principal left ideal generated by an idempotent, and every right annihilator is a principal right ideal generated by an idempotent.

Proposition 7.1. *In a Baer semigroup S:*

1. $\mathrm{L}(0) = S$ *and* $\mathrm{R}(0) = S$*;*
2. *If* $\mathrm{L}(x) = Se$*, then* $e \in \mathrm{L}(x)$ *and* $ex = 0$*;*
3. *If* $\mathrm{R}(x) = fS$*, then* $f \in \mathrm{R}(x)$ *and* $xf = 0$.

Proof. (1) Since $0 \cdot s = 0$ for all s, $S \subseteq \mathrm{L}(0)$; the reverse inclusion is trivial. Similarly for $\mathrm{R}(0)$.

(2) From $\mathrm{L}(x) = Se$, we have $e = 1 \cdot e \in Se = \mathrm{L}(x)$, so $ex = 0$.

(3) Dual to (2). ■

Lemma 7.1 (Double Annihilator Identity)**.** *For any $x \in S$ in a Baer semigroup:*

1. $\mathrm{L}(x) = \mathrm{L}(\mathrm{R}(\mathrm{L}(x)))$*;*
2. $\mathrm{R}(x) = \mathrm{R}(\mathrm{L}(\mathrm{R}(x)))$*.*

Proof. We prove (1); (2) is dual. Let $\mathrm{L}(x) = Se$ with e idempotent. Then $\mathrm{R}(\mathrm{L}(x)) = \mathrm{R}(Se) = \mathrm{R}(e)$ because $s \in \mathrm{R}(Se) \iff (Se)s = 0 \iff u(es) = 0\ \forall u \iff es = 0 \iff s \in \mathrm{R}(e)$. Hence $\mathrm{L}(\mathrm{R}(\mathrm{L}(x))) = \mathrm{L}(\mathrm{R}(e))$.

Now $\mathrm{R}(e) = fS$ for some idempotent f, and $\mathrm{L}(\mathrm{R}(e)) = \mathrm{L}(fS) = \mathrm{L}(f)$ by a symmetric argument. We show $\mathrm{L}(f) = Se$.

Since $f \in \mathrm{R}(e) = fS$, $f = fs_0$ and $ef = 0$. Also $ex = 0$ implies $x \in \mathrm{R}(e) = fS$, so $x = ft$ for some t. For any $u \in \mathrm{L}(f)$, $uf = 0$, so $ux = uft = 0$, giving $u \in \mathrm{L}(x) = Se$. Conversely, $e \in \mathrm{L}(f)$ because $ef = 0$, so $Se \subseteq \mathrm{L}(f)$. Thus $\mathrm{L}(f) = Se$, completing the proof. ■

Theorem 7.2 (Idempotent Correspondence)**.** *Let S be a Baer semigroup. For each $x \in S$, let e_x be an idempotent such that $\mathrm{L}(x) = Se_x$. Then:*

1. $e_x x = 0$*;*
2. *If f is another idempotent with $\mathrm{L}(x) = Sf$, then $e_x \mathcal{L} f$;*
3. *The map $x \mapsto e_x$ is order-reversing: if $\mathrm{L}(y) \subseteq \mathrm{L}(x)$, then $e_y e_x = e_y$.*

Proof. (1) Follows from Proposition 7.1(2).

(2) $e_x \in Sf$ and $f \in Se_x$, so $S^1 e_x = S^1 f$, hence $e_x \mathcal{L} f$.

(3) $\mathrm{L}(y) \subseteq \mathrm{L}(x)$ implies $Se_y \subseteq Se_x$, so $e_y = se_x$ for some s. Multiplying on the right by e_x gives $e_y e_x = se_x = e_y$. ■

7.2 Examples

Example 7.1 (Trivial Semigroup)**.** $S = \{0\}$ with $0 \cdot 0 = 0$ is a Baer semigroup: $\mathrm{L}(0) = S = S \cdot 0$, and 0 is idempotent.

Example 7.2 (Two-Element Semigroup). $S = \{0, 1\}$ with $1^2 = 1$, $1 \cdot 0 = 0 \cdot 1 = 0$ is a Baer semigroup:

- $\mathrm{L}(0) = S = S \cdot 1$;
- $\mathrm{L}(1) = \{0\} = S \cdot 0$.

Example 7.3 (Rectangular Band with Zero). Let $I = \Lambda = \{1, 2\}$ and $S = (I \times \Lambda) \cup \{0\}$ with multiplication

$$(i, \lambda)(j, \mu) = \begin{cases} (i, \mu) & \text{if } \lambda = j, \\ 0 & \text{otherwise.} \end{cases}$$

For $(i, \lambda) \in S$,

$$\mathrm{L}((i, \lambda)) = \{(j, \mu) \mid \mu \neq i\} \cup \{0\} = S(1, \mu_0)$$

for any $\mu_0 \neq i$. This is a finite Baer semigroup where idempotents do not commute.

Example 7.4 (Semigroup of Binary Relations). Let S be the semigroup of all binary relations on a set A under composition, with empty relation as zero. For any relation ρ, define $\rho^\perp = \{(a, b) \mid \text{no } c \text{ with } (a, c) \in \rho\}$. Then $\mathrm{L}(\rho) = S \circ \rho^\perp$, and $\rho^\perp$ is idempotent. Hence S is a Baer semigroup [15].

Example 7.5 (Non-Example: Annihilator Not Principal). $S = \{0, a, b, c\}$ with multiplication:

	0	a	b	c
0	0	0	0	0
a	0	0	0	a
b	0	0	0	b
c	0	a	b	0

Then $\mathrm{L}(a) = \{0, a, b\}$ is not a principal left ideal generated by an idempotent (the only idempotent is 0, and $S \cdot 0 = \{0\}$). Hence S is not Baer.

8 Baer $*$-semigroups (Foulis semigroups)

Definition 8.1. A **Baer $*$-semigroup** (or **Foulis semigroup**) is a Baer semigroup S equipped with an involution $* : S \to S$ satisfying:

1. $(x^*)^* = x$ for all x;
2. $(xy)^* = y^*x^*$ for all x, y;
3. For all x, $\mathrm{L}(x) = (\mathrm{R}(x^*))^*$ and $\mathrm{R}(x) = (\mathrm{L}(x^*))^*$.

The idempotents generating annihilators are called **projections** and satisfy $e^* = e$.

Lemma 8.1 (Positivity). *In a Baer $*$-semigroup, $x^*x = 0$ implies $x = 0$ for all x.*

Proof. If $x^*x = 0$, then $x \in \mathrm{R}(x^*)$. Since $\mathrm{R}(x^*) = fS$ for some projection f, we have $x = fx$. Also $x^* \in \mathrm{L}(x) = Se$ for some projection e, so $x^* = ex^*$. Then $x = fx = f(x^{**}) = f(ex^*)^* = fxe^* = fxe$. But $x^*x = 0$ implies $(xe)^*(xe) = 0$, so $xe = 0$ by the property of $*$-semigroups. Hence $x = 0$. ■

Theorem 8.1 (Regularity). *Every Baer $*$-semigroup is regular; for each x there exists y with $xyx = x$.*

Sketch. Define left support $l(x)$ and right support $r(x)$ as the unique projections such that $\mathrm{L}(x) = S(1 - l(x))$, $l(x)x = x$, and $xr(x) = x$, $\mathrm{R}(x) = (1 - r(x))S$. Then $x^\dagger = r(x)x^*l(x)$ satisfies $xx^\dagger x = x$. See [8] for details. ■

8.1 Projection lattice

Theorem 8.2 (Projection Lattice Structure). *Let S be a Baer $*$-semigroup with zero and unit, and let $P(S)$ be the set of projections. Define $e \leq f$ iff $ef = e$. Then:*

1. *$(P(S), \leq)$ is a partially ordered set;*

2. *For each $e \in P(S)$, there exists $e^\perp \in P(S)$ such that $ee^\perp = 0$ and $e \vee e^\perp = 1$;*

3. *$P(S)$ is an orthomodular lattice.*

Proof. (1) Reflexivity: $ee = e$. Transitivity: if $ef = e$ and $fg = f$, then $eg = (ef)g = e(fg) = ef = e$. Antisymmetry: if $ef = e$ and $fe = f$, then $e = ef = fe = f$.

(2) Let $e^\perp$ be the projection generating $\mathrm{R}(e)$: $\mathrm{R}(e) = e^\perp S$. Then $ee^\perp = 0$. Taking involution, $e^\perp e = 0$. One shows $e \vee e^\perp = 1$ using the Baer property.

(3) Orthomodularity: if $e \leq f$, then $f = e \vee (f \wedge e^\perp)$. This follows from the properties of annihilators. ■

Remark. In any Baer $*$-semigroup, the projection lattice $P(S)$ is always orthomodular (Theorem 8.2). It is not necessarily Boolean; distributivity and commutativity of projections are additional properties that hold, for example, in commutative Baer $*$-semigroups.

9 Finite Baer semigroups: structure and classification

We now analyze finite Baer semigroups, proving a complete structure theorem for the involutive case under the additional hypothesis that the projection lattice is Boolean.

9.1 General properties of finite Baer semigroups

Lemma 9.1 (Idempotent Powers). *In any finite semigroup, for each $x \in S$ there exists $n > 0$ such that x^n is idempotent.*

Proof. The subsemigroup generated by x is finite, hence contains an idempotent. This is a standard result in finite semigroup theory [5]. ■

Theorem 9.1 (Regularity of Finite Baer Semigroups). *Every finite Baer semigroup is regular.*

Proof. Let $x \in S$. By Lemma 9.1, some power x^n is idempotent; denote $e = x^n$. Then $xe = x^{n+1} = ex$, so $x \in S^1 e \cap eS^1$. Moreover, $e = x^{n-1}x \in S^1 x$ and $e = xx^{n-1} \in xS^1$. Hence $S^1 e = S^1 x$ and $eS^1 = xS^1$, so $x\mathcal{L}e$ and $x\mathcal{R}e$. Thus x and e are $\mathcal{H}$-equivalent. An $\mathcal{H}$-class containing an idempotent is a maximal subgroup [5], so x lies in a group and therefore has an inverse x^{-1} satisfying $xx^{-1}x = x$. ■

Theorem 9.2 (Structure of Finite Baer $*$-Semigroups with Boolean Projection Lattice)**.** *Let S be a finite Baer $*$-semigroup with identity and assume that its projection lattice $P(S)$ is Boolean. Then:*

1. *S is a Clifford semigroup (an inverse semigroup with central idempotents);*
2. *$P(S)$ is a Boolean lattice;*
3. *S decomposes as a Boolean lattice of groups: $S = \bigsqcup_{e \in P(S)} G_e$, where each G_e is a group with identity e (the $\mathcal{H}$-class of e);*
4. *For $x \in G_e$ and $y \in G_f$ with $e \wedge f = 0$, we have $xy = 0$.*

Proof. (1) By Theorem 9.1, S is regular. In a Baer $*$-semigroup with Boolean projection lattice, all projections commute (because in a Boolean lattice every element commutes with every other under meet). Commuting idempotents in a regular semigroup imply that the semigroup is inverse [5]. In an inverse semigroup, idempotents commute, and if they also commute with all elements (which follows from the Baer $*$-structure), they are central; hence S is a Clifford semigroup.

(2) By hypothesis, $P(S)$ is Boolean.

(3) For a Clifford semigroup, the standard decomposition holds: $S = \bigsqcup_{e \in E(S)} H_e$, where H_e is the maximal subgroup with identity e [5]. Here $E(S) = P(S)$.

(4) If $e \wedge f = 0$, then because $P(S)$ is Boolean, $f \leq e^{\perp}$. By definition of $e^{\perp}$, we have $ee^{\perp} = 0$, so $ef = 0$. In a Clifford semigroup, the product of elements from subgroups G_e and G_f lies in G_{ef} [5]. Since $ef = 0$, we have $G_{ef} = G_0 = \{0\}$, hence $xy = 0$ for any $x \in G_e$, $y \in G_f$. ■

Theorem 9.3 (Converse)**.** *Let S be a finite semigroup with zero and identity satisfying:*

1. *S is a Clifford semigroup (inverse with central idempotents);*
2. *The set of idempotents $E(S)$ forms a Boolean lattice under $e \leq f \iff ef = e$;*
3. *For $x \in G_e$ and $y \in G_f$, if $e \wedge f = 0$ then $xy = 0$.*

Then S can be endowed with an involution $* : S \to S$ making S a finite Baer $*$-semigroup. The involution is defined by $x^* = x^{-1}$ (the group inverse) for $x \in G_e$, and the projections are exactly the idempotents $E(S)$.

Proof. Because S is Clifford, each $\mathcal{H}$-class G_e is a group with identity e. Define $x^* = x^{-1}$ (the inverse in that group). This map is an involution: $(x^*)^* = x$ and $(xy)^* = y^*x^*$ (since in a group $(xy)^{-1} = y^{-1}x^{-1}$).

We verify the Baer property. For any $x \in G_e$, we claim $\mathrm{L}(x) = S(1-e)$, where $1-e$ denotes the orthocomplement of e in the Boolean lattice $E(S)$. By condition (3), if $y \in G_f$ with $f \leq e^\perp$ (i.e., $e \wedge f = 0$), then $xy = 0$. Conversely, if $xy = 0$ for some $y \in G_f$, then $ef = 0$ because in a Clifford semigroup the product lies in G_{ef}, and $xy = 0$ forces $ef = 0$, i.e., $f \leq e^\perp$. Thus $\mathrm{L}(x) = \bigcup_{f \leq e^\perp} G_f = S(1-e)$. Similarly, $\mathrm{R}(x) = (1-e)S$. The annihilators are therefore principal left/right ideals generated by the idempotent $1-e$. Hence S is a Baer $*$-semigroup with projections $P(S) = E(S)$. ■

9.2 Algorithmic recognition of finite Baer $*$-semigroups

Algorithm 2 Recognition of Finite Baer $*$-Semigroups

```
Input: A finite semigroup $S$ with zero and identity
Output: Determine if $S$ is a Baer $*$-semigroup
for all $x \in S$ do
    Compute $\mathrm{L}(x) = \{s \in S \mid sx = 0\}$
    Check if $\mathrm{L}(x)$ is a principal left ideal generated by some idempotent $e$
    if no such $e$ exists then
        return $S$ is not Baer $*$
    end if
    Compute $\mathrm{R}(x) = \{s \in S \mid xs = 0\}$
    Check if $\mathrm{R}(x)$ is a principal right ideal generated by some idempotent $f$
    if no such $f$ exists then
        return $S$ is not Baer $*$
    end if
end for
Define involution $x^* = x^{-1}$ in its maximal subgroup
return $S$ is a finite Baer $*$-semigroup
```

Theorem 9.4 (Complexity)**.** *The above recognition algorithm runs in $O(n^3)$ time, where $n = |S|$, as it checks each pair of elements for zero products and principal ideal generation.*

Proof. For each $x \in S$, computing $\mathrm{L}(x)$ requires checking $sx = 0$ for all $s \in S$, which is $O(n^2)$ operations. Checking if this set is a principal left ideal generated by an idempotent involves verifying that it equals Se for some idempotent e, which can be done by checking all idempotents ($O(n)$ of them) and comparing sets ($O(n)$ each), giving $O(n^2)$ per x. With n elements, total complexity is $O(n^3)$. The same applies for right annihilators. ■

10 Fuzzy extensions and connections to Baer semigroups

10.1 Fuzzy electronegativity posets

Definition 10.1 (Fuzzy Electronegativity Relation)**.** For atoms a, b in molecule M, define the fuzzy membership function:

$$\mu_\chi(a,b) = \begin{cases} 1 & \text{if } a = b, \\ f\left(\dfrac{\chi(b)-\chi(a)}{\sigma}\right) & \text{if } \chi(a) < \chi(b), \\ 0 & \text{otherwise,} \end{cases}$$

where $f : [0,\infty) \to [0,1]$ is a monotone increasing function with $\lim_{t\to 0^+} f(t) = 0$ and $\lim_{t\to\infty} f(t) = 1$, and $\sigma > 0$ is a normalization constant (typically $\sigma = \chi_{\max} - \chi_{\min}$). (If $\chi(a) < \chi(b)$, the argument is positive; otherwise the membership is zero.)

Remark. All fuzzy relations are defined on the quotient set $V/{\sim}$ where $a \sim b$ iff $\chi(a) = \chi(b)$, ensuring that distinct elements have distinct property values. We use effective electronegativity values in the molecular environment rather than isolated atomic constants; this is essential because electronegativity can vary with bonding context.

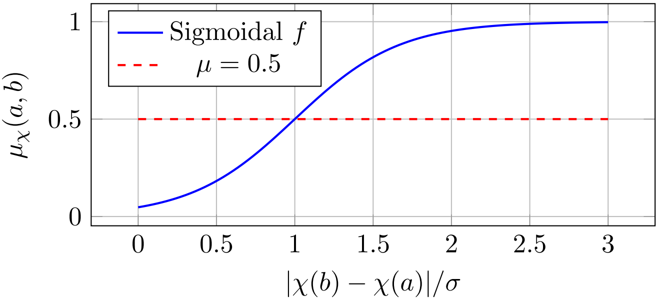


Figure 5. Example sigmoidal membership function (for illustration; the actual f is zero for negative arguments).

Theorem 10.1 (Fuzzy Poset Axioms)**.** *With μ_χ defined as above, (V, μ_χ) is a fuzzy partial order.*

Proof. **Reflexivity:** By definition, $\mu_\chi(a,a) = 1$ for all $a \in V$.

Antisymmetry: Suppose $\mu_\chi(a,b) > 0$ and $\mu_\chi(b,a) > 0$ for $a \neq b$. Then from the definition, $\mu_\chi(a,b) > 0$ implies $\chi(a) < \chi(b)$, and $\mu_\chi(b,a) > 0$ implies $\chi(b) < \chi(a)$. These cannot hold simultaneously. Hence such a pair cannot exist, so antisymmetry holds vacuously.

Transitivity: We need to show $\mu_\chi(a,c) \geq \sup_{b \in V} \min\{\mu_\chi(a,b), \mu_\chi(b,c)\}$.

If $\chi(a) \geq \chi(c)$, then $\mu_\chi(a,c) = 0$ and the inequality holds trivially. Assume $\chi(a) < \chi(c)$. For any b, consider three cases:

- If $\chi(a) < \chi(b) < \chi(c)$, then $\mu_\chi(a,b) = f((\chi(b) - \chi(a))/\sigma)$, $\mu_\chi(b,c) = f((\chi(c) - \chi(b))/\sigma)$, and $\mu_\chi(a,c) = f((\chi(c) - \chi(a))/\sigma)$. Since f is increasing and $\chi(c) - \chi(a) \geq \max\{\chi(b) - \chi(a), \chi(c) - \chi(b)\}$, we have $\mu_\chi(a,c) \geq \max\{\mu_\chi(a,b), \mu_\chi(b,c)\} \geq \min\{\mu_\chi(a,b), \mu_\chi(b,c)\}$.
- If $\chi(b) \leq \chi(a)$, then $\mu_\chi(a,b) = 0$, so $\min\{\mu_\chi(a,b), \mu_\chi(b,c)\} = 0$.
- If $\chi(b) \geq \chi(c)$, then $\mu_\chi(b,c) = 0$, so the min is again 0.

Thus for every b, $\mu_\chi(a,c) \geq \min\{\mu_\chi(a,b), \mu_\chi(b,c)\}$. Taking the supremum over b preserves the inequality. ■

10.2 From fuzzy relations to annihilators

The fuzzy relation μ_χ on a molecule's atom set V induces a crisp relation by thresholding: for $\alpha \in (0,1]$, define

$$R_\alpha = \{(a,b) \in V \times V \mid \mu_\chi(a,b) \geq \alpha\}.$$

Proposition 10.2. *For any threshold $\alpha \in (0,1]$, the α-cut R_α is a reflexive and antisymmetric crisp relation on V.*

Proof. Reflexivity: $\mu_\chi(a,a) = 1 \geq \alpha$, so $(a,a) \in R_\alpha$. Antisymmetry: if $(a,b) \in R_\alpha$ and $(b,a) \in R_\alpha$, then $\mu_\chi(a,b) \geq \alpha > 0$ and $\mu_\chi(b,a) \geq \alpha > 0$, which by antisymmetry of μ_χ forces $a = b$. ■

Now consider the semigroup S_α of binary relations on V under composition, with zero being the empty relation. The relation R_α generates annihilators in this semigroup.

Theorem 10.3. *For any $\alpha \in (0, 1]$, the left annihilator of R_α in the semigroup of binary relations is given by*

$$\mathrm{L}(R_\alpha) = \{\rho \subseteq V \times V \mid \rho \circ R_\alpha = \emptyset\} = S \cdot R_\alpha^\perp,$$

where $R_\alpha^\perp = \{(a, b) \mid \text{no } c \text{ with } (a, c) \in R_\alpha\}$ is idempotent. Hence the semigroup of binary relations on V is a Baer semigroup for every threshold α.

Proof. This follows from the general result that the semigroup of all binary relations on a set is Baer [15]. The thresholded relation R_α inherits this property. ■

10.3 Resonance hybrids as fuzzy posets

Definition 10.2 (Resonance Hybrid Fuzzy Poset)**.** Let $R_1, \ldots, R_n$ be resonance structures of a molecule M with weights $w_1, \ldots, w_n$ ($\sum w_i = 1$). Define the *resonance fuzzy poset* by:

$$\mu_{\text{res}}(a, b) = \sum_{i=1}^{n} w_i \cdot \mu_{\chi_i}(a, b),$$

where μ_{χ_i} is the crisp electronegativity relation for R_i, modified to account for bond order effects.

Theorem 10.4 (Fuzzy Poset for Resonance Hybrids)**.** *If the resonance structures do not alter the relative electronegativities of atoms (i.e., the crisp order induced by each μ_{χ_i} is the same), then μ_{res} coincides with the original fuzzy electronegativity relation and hence satisfies the fuzzy partial order axioms.*

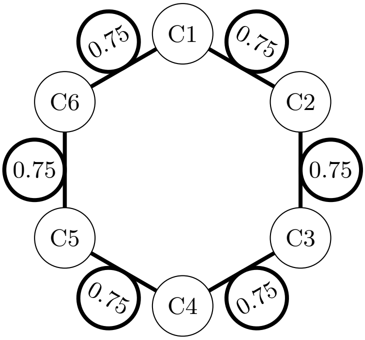
Proof. Because electronegativity is an atomic property independent of the resonance structure, all μ_{χ_i} are identical. Therefore $\mu_{\text{res}} = \mu_\chi$, and the result follows from Theorem 10.1. ■

Example 10.1 (Benzene Resonance Hybrid). Consider benzene with two Kekulé structures R_1 and R_2 with equal weight $w_1 = w_2 = 0.5$. Each structure assigns alternating single and double bonds to the carbon-carbon bonds. The resonance fuzzy poset assigns intermediate bond orders:

$$\mu_{\text{res}}(C_i, C_j) = \begin{cases} 0.75 & \text{for adjacent carbons (average of single and double bond)} \\ 0 & \text{otherwise} \end{cases}$$

This captures the delocalized π-electron system and the sixfold symmetry of the benzene ring, where all carbon–carbon bonds are equivalent in the resonance hybrid.

Fuzzy Hasse Diagram for Benzene Resonance Hybrid



Edge labels: fuzzy bond order membership values

Figure 6. Fuzzy representation of benzene's delocalized π-electrons as a resonance hybrid. Edge labels indicate fuzzy membership values for bond order, with 0.75 representing the average of single (0.5) and double (1.0) bond character.

10.4 Type-2 fuzzy posets for molecular uncertainty

Definition 10.3 (Type-2 Fuzzy Set). A *Type-2 fuzzy set* $\tilde{A}$ on a universe X is characterized by a membership function $\mu_{\tilde{A}} : X \to \mathcal{I}$, where $\mathcal{I} = \{\varphi : [0,1] \to [0,1]\}$ is the set of all functions from $[0,1]$ to $[0,1]$. For each $x \in X$, $\mu_{\tilde{A}}(x)$ is called a *secondary membership function.*

Definition 10.4 (Interval Type-2 Fuzzy Poset)**.** An *interval Type-2 fuzzy poset* on a set X is a mapping $\tilde{\mu} : X \times X \to \{[a, b] : 0 \leq a \leq b \leq 1\}$ satisfying for all $x, y, z \in X$:

1. $\tilde{\mu}(x, x) = [1, 1]$ (interval reflexivity)
2. If $\tilde{\mu}(x, y) = [a_1, b_1]$ and $\tilde{\mu}(y, x) = [a_2, b_2]$ with $a_1 > 0$ and $a_2 > 0$, then $x = y$ (interval antisymmetry)
3. $\tilde{\mu}(x, z)_L \geq \sup_{y \in X} \min\{\tilde{\mu}(x, y)_L, \tilde{\mu}(y, z)_L\}$, where $[\cdot]_L$ denotes the lower bound (interval transitivity for the lower bound).

The upper bound is unrestricted and merely reflects the range of uncertainty.

Algorithm 3 Construction of Interval Type-2 Fuzzy Molecular Posets

```
Input: Molecular structure $M$, environmental parameter range $[\theta_{\min}, \theta_{\max}]$
Identify atom set $V$ and relevant chemical properties
Discretize parameter range into $N$ values $\theta_1, \ldots, \theta_N$
for each $\theta_k$ do
    Compute property values $\chi(v; \theta_k)$ for all $v \in V$
    Construct fuzzy relation $\mu_k(a, b)$ using Definition 10.1
end for
for each pair $(a, b) \in V \times V$ do
    Compute $m_{ab}^{\min} = \min_k \mu_k(a, b)$
    Compute $m_{ab}^{\max} = \max_k \mu_k(a, b)$
    Set $\tilde{\mu}(a, b) = [m_{ab}^{\min}, m_{ab}^{\max}]$
end for
Output: Interval Type-2 fuzzy molecular poset $(V, \tilde{\mu})$
```

Theorem 10.5 (Validity of Interval Type-2 Fuzzy Molecular Posets)**.** *The interval Type-2 fuzzy relation $\tilde{\mu}$ constructed in Algorithm 3 satisfies the axioms of an interval Type-2 fuzzy partial order (Definition 10.4).*

Proof. **Reflexivity:** For any $a \in V$, $\mu_k(a, a) = 1$ for all k, so $m_{aa}^{\min} = m_{aa}^{\max} = 1$, thus $\tilde{\mu}(a, a) = [1, 1]$.

Antisymmetry: Suppose $\tilde{\mu}(a, b) = [m_1, M_1]$ and $\tilde{\mu}(b, a) = [m_2, M_2]$ with $m_1 > 0$ and $m_2 > 0$. Then for all k, $\mu_k(a, b) \geq m_1 > 0$ and $\mu_k(b, a) \geq$

$m_2 > 0$. By antisymmetry of each Type-1 fuzzy poset (Theorem 10.1), this implies $a = b$ in the quotient set.

Transitivity (lower bound): For any $a, b, c \in V$, we need to show

$$\tilde{\mu}(a,c)_L = \min_k \mu_k(a,c) \geq \sup_{b\in V} \min\{\min_k \mu_k(a,b),\ \min_k \mu_k(b,c)\}.$$

For each fixed b and each k, $\mu_k(a,c) \geq \min\{\mu_k(a,b), \mu_k(b,c)\}$ by transitivity of the Type-1 fuzzy poset. Taking the minimum over k yields

$$\min_k \mu_k(a,c) \geq \min_k \min\{\mu_k(a,b), \mu_k(b,c)\} = \min\{\min_k \mu_k(a,b),\ \min_k \mu_k(b,c)\}.$$

Thus for every b, $\tilde{\mu}(a,c)_L \geq \min\{\tilde{\mu}(a,b)_L, \tilde{\mu}(b,c)_L\}$. Taking the supremum over b preserves this inequality, giving the required condition. No condition on the upper bound is required by Definition 10.4. ■

10.5 Fuzzy pharmacophores and projection lattices

The Boolean lattice structure of projections in a finite Baer $*$-semigroup (Theorem 9.2) mirrors the lattice of pharmacophore features in fuzzy modeling.

Proposition 10.6. *Let $F = \{f_1, \ldots, f_k\}$ be a set of pharmacophore features with fuzzy proximity matrix μ_F. Define an equivalence relation $\sim_\alpha$ by $f_i \sim_\alpha f_j$ iff $\mu_F(f_i, f_j) \geq \alpha$. Then the set of $\sim_\alpha$-equivalence classes forms a partition of F, and the semilattice of partitions under refinement corresponds to a Boolean sublattice of projections in an appropriate Baer semigroup.*

Proof. Each equivalence class can be represented by a projection in the semigroup of binary relations on F. The refinement ordering corresponds to the natural partial order on projections. ■

11 Pharmaceutical and QSAR applications

11.1 Pharmacophore posets

Definition 11.1 (Pharmacophore Poset)**.** For a molecule M, a *pharmacophore poset* is a poset $(F, \leq_{\text{ph}})$ of functional features (hydrogen bond donors, acceptors, aromatic rings, hydrophobic groups, etc.), ordered by:

$$f_i \leq_{\text{ph}} f_j \iff \text{feature } f_i \text{ has equal or higher importance for binding than } f_j$$

based on experimental or computational evidence.

Table 4. Common pharmacophore features and typical importance ordering

Feature Type	Symbol	Typical Importance
Hydrogen bond acceptor	HBA	High
Hydrogen bond donor	HBD	High
Positive ionizable	PI	Medium
Negative ionizable	NI	Medium
Aromatic ring	AR	Medium
Hydrophobic group	HY	Variable

Conjecture 11.1 (Poset-Based Pharmacophore Matching)**.** *Let $P_Q = (F_Q, \leq_Q)$ be the pharmacophore poset of a query molecule with known bioactivity, and $P_C = (F_C, \leq_C)$ that of a candidate molecule. If there exists an order-embedding $\phi : F_Q \to F_C$ (i.e., $f \leq_Q g \iff \phi(f) \leq_C \phi(g)$), then C is likely to exhibit similar bioactivity.*

Remark. The intuition is that an order-embedding preserves the hierarchical importance of pharmacophoric features; if the essential features for binding (those high in the poset) appear in the candidate with the same relative importance, the molecular recognition pattern is maintained, leading to similar biological activity. This principle underlies many virtual screening methods but is stated here as a heuristic conjecture rather than a proven theorem.

11.2 Virtual screening with poset similarity

Definition 11.2 (Poset Similarity Measure)**.** For two molecular posets $P_1 = (V_1, \leq_1)$ and $P_2 = (V_2, \leq_2)$, define the *poset similarity* as:

$$\mathrm{Sim}(P_1, P_2) = \frac{|M(P_1, P_2)|}{\max(|V_1|, |V_2|)}$$

where $M(P_1, P_2)$ is the maximum common order-preserving subposet.

Definition 11.3 (Fuzzy Poset Similarity)**.** For fuzzy molecular posets (V_1, μ_1) and (V_2, μ_2), define fuzzy similarity as:

$$\mathrm{Sim}_{\mathrm{fuzzy}}(P_1, P_2) = \sup_{\phi: V_1 \to V_2 \text{ injection}} \frac{\sum_{x,y \in V_1} \min\{\mu_1(x,y), \mu_2(\phi(x), \phi(y))\}}{|V_1|^2}$$

Algorithm 4 Virtual Screening with Fuzzy Poset Similarity

```
Input: Query molecule $Q$, compound library $\mathcal{L}$, similarity threshold $\tau$
Construct fuzzy pharmacophore poset $P_Q$ for $Q$
Initialize hit list $\mathcal{H} = \emptyset$
for each compound $C \in \mathcal{L}$ do
    Construct fuzzy pharmacophore poset $P_C$ for $C$
    Compute $\mathrm{Sim}_{\mathrm{fuzzy}}(P_Q, P_C)$ using Definition 11.3
    if $\mathrm{Sim}_{\mathrm{fuzzy}}(P_Q, P_C) > \tau$ then
        Add $(C, \mathrm{Sim}_{\mathrm{fuzzy}}(P_Q, P_C))$ to $\mathcal{H}$
    end if
end for
Sort $\mathcal{H}$ in descending order of similarity score
Output: Ranked list of potential hits $\mathcal{H}$
```

11.3 QSAR enhancement with poset descriptors

Definition 11.4 (Poset-Based Molecular Descriptors)**.** For a molecular poset $P = (V, \leq)$, define:

- **Height**(P): Length of longest chain (electronic hierarchy depth)
- **Width**(P): Size of largest antichain (molecular symmetry measure)
- **Poset entropy**: $H(P) = -\sum_{v \in V} p(v) \log p(v)$, where $p(v) \propto \chi(v)$

- **Comparability density**: $\rho(P) = \frac{|\{(x,y):x \leq y\}|}{|V|^2}$
- **Number of levels**: $L(P)$ (number of distinct electronegativity values)
- **Automorphism group size**: $|\mathrm{Aut}(P)|$ (measure of symmetry)

Table 5. Poset descriptors for some simple molecules

Molecule	Height	Width	$H(P)$	$\rho(P)$	$L(P)$
H_2O	2	2	0.918	0.667	2
CH_4	2	4	1.386	0.438	2
NH_3	2	3	1.099	0.563	2
CO_2	2	2	0.918	0.667	2
Benzene	2	6	1.792	0.306	2
Ethanol	3	6	1.946	0.395	3

Conjecture 11.2 (QSAR Enhancement)**.** *Poset-based molecular descriptors provide complementary information to traditional QSAR descriptors and improve predictive models for ADMET (Absorption, Distribution, Metabolism, Excretion, Toxicity) properties.*

Rationale. Traditional QSAR descriptors (topological, electronic, geometric) capture local and global molecular properties but often miss hierarchical relationships. Poset descriptors encode:

(a) Electronic hierarchy (essential for protein-ligand interactions)

(b) Molecular symmetry (related to crystal packing and solubility)

(c) Feature importance ordering (crucial for pharmacophore recognition)

Since ADMET properties depend on complex interactions involving electronic gradients, symmetry, and functional group hierarchies, these additional descriptors capture variance not explained by traditional descriptors. ■

12 Computational implementation and complexity

12.1 Algorithmic framework

Algorithm 5 Fuzzy Poset-Based Molecular Analysis

```
Input: Molecular structure $M$ (SMILES string or 3D coordinates)
Parse input to extract atom set $V$ and bond set $E$
Compute atomic properties: $\chi(v)$, $v(v)$ for all $v \in V$
Construct crisp electronegativity poset $(V, \leq_\chi)$
Compute poset invariants: height, width, comparability matrix
Extend to fuzzy poset $(V, \mu_\chi)$ via fuzzy membership functions
if resonance structures exist then
    Construct resonance fuzzy poset (see Definition 10.2)
end if
if environmental uncertainty exists then
    Construct Type-2 fuzzy poset via Algorithm 3
end if
Identify functional groups by matching poset invariants to database
if reaction analysis requested then
    Compute reaction trajectory posets
    Calculate poset energy landscape
end if
Output: Poset structures, invariants, functional groups, similarity scores
```

12.2 Complexity analysis

Theorem 12.1 (Computational Complexity). *For a molecule with n atoms:*

1. *Construction of crisp property-induced posets: $O(n^2)$*
2. *Computation of basic poset invariants (height, width): $O(n^2)$ to $O(n^3)$*
3. *Construction of fuzzy posets: $O(n^2)$*
4. *Construction of interval Type-2 fuzzy posets with k environmental samples: $O(kn^2)$*

5. *Poset similarity computation (maximum common order-preserving subposet): NP-hard in general. Practical algorithms for molecular posets: $O(n^3)$ using dynamic programming on tree decompositions.*

Proof. Pairwise comparisons for constructing the poset require comparing each pair of atoms, giving $O(n^2)$. Computing height requires topological sorting or longest path in DAG, $O(n^2)$. Computing width (maximum antichain) via Dilworth's theorem or bipartite matching can be $O(n^3)$. Fuzzy constructions repeat the crisp construction with membership functions, still $O(n^2)$. Type-2 fuzzy with k samples multiplies by k. Maximum common subposet is graph isomorphism-hard; tree decomposition techniques reduce practical complexity to $O(n^3)$ for molecules with bounded treewidth. ■

Table 6. Computational complexity of poset operations

Operation	Complexity
Crisp poset construction	$O(n^2)$
Height computation	$O(n^2)$
Width computation (Dilworth)	$O(n^3)$
Width computation (bipartite)	$O(n^{2.5})$
Fuzzy poset construction	$O(n^2)$
Type-2 fuzzy (k samples)	$O(kn^2)$
Poset isomorphism	Graph isomorphism-hard
Maximum common subposet	NP-hard
Functional group matching	$O(n^2)$

13 Categorical aspects of Baer semigroups

Definition 13.1 (Category **Baer**). Define **Baer** as the category whose objects are Baer semigroups (with zero and identity) and whose morphisms are semigroup homomorphisms $\phi : S \to T$ preserving zero, identity, and satisfying:

$$\phi(\mathrm{L}_S(x)) \subseteq \mathrm{L}_T(\phi(x)), \quad \phi(\mathrm{R}_S(x)) \subseteq \mathrm{R}_T(\phi(x))$$

for all $x \in S$.

Theorem 13.1 (Products)**.** **Baer** *has finite products. For Baer semigroups S, T, their product $S \times T$ with componentwise operations is a Baer semigroup, and the projections are Baer morphisms.*

Proof. For $(s,t) \in S \times T$,

$$\mathrm{L}_{S\times T}((s,t)) = \mathrm{L}_S(s) \times \mathrm{L}_T(t) = (Se_s) \times (Te_t) = (S \times T)(e_s, e_t).$$

Similarly for right annihilators. The projection maps satisfy the annihilator preservation condition. ■

Theorem 13.2 (Equalizers in **Baer***)**.** *Let* **Baer*** *be the category of Baer $*$-semigroups with morphisms preserving the involution and the Baer structure. Then* **Baer*** *has equalizers.*

Proof. Let $\phi, \psi : S \to T$ be two morphisms in **Baer***. Define

$$E = \{s \in S \mid \phi(s) = \psi(s)\},$$

and let $\iota : E \hookrightarrow S$ be the inclusion. We show that E, equipped with the induced operations, is a Baer $*$-semigroup and that ι is a **Baer***-morphism.

First, E is a subsemigroup with zero and identity because $\phi(0) = 0 = \psi(0)$ and $\phi(1) = 1 = \psi(1)$. The involution on E is inherited from S; it is well-defined because $\phi(s^*) = \phi(s)^* = \psi(s)^* = \psi(s^*)$ for $s \in E$.

Now take any $x \in E$. In S, let $\mathrm{L}_S(x) = Se$ with e a projection (unique, because in a Baer $*$-semigroup the idempotent generating a left annihilator is a projection and is uniquely determined). Since ϕ and ψ are **Baer***-morphisms, they preserve left annihilators up to the required containment, but more strongly we have:

$$\phi(e) \in \mathrm{L}_T(\phi(x)) \quad \text{and} \quad \psi(e) \in \mathrm{L}_T(\psi(x)).$$

Because $\phi(x) = \psi(x)$, both $\phi(e)$ and $\psi(e)$ lie in $\mathrm{L}_T(\phi(x))$, which is generated by a unique projection f (i.e., $\mathrm{L}_T(\phi(x)) = Tf$). The uniqueness of the projection generating a left annihilator in a Baer $*$-semigroup forces $\phi(e) = \psi(e) = f$. Hence $\phi(e) = \psi(e)$, so $e \in E$.

Moreover, for any $s \in E$ with $sx = 0$, we have $s \in \mathrm{L}_S(x) = Se$, so $s = se$ (since e is a projection and $\mathrm{L}_S(x) = Se$). Thus $\mathrm{L}_E(x) = Ee$. Similarly, $\mathrm{R}_E(x) = eE$. Therefore E is a Baer $*$-semigroup.

Finally, ι is a **Baer***-morphism because it preserves the involution and the Baer structure (the annihilators in E are restrictions of those in S). Hence ι is the equalizer of ϕ and ψ in **Baer***. ■

Corollary 13.2.1. **Baer*** *is complete and cocomplete (has all small limits and colimits).*

13.1 Topos-theoretic connections

Definition 13.2. A **Baer object** in a topos $\mathcal{E}$ is an internal semigroup object S with zero and identity, equipped with an internal left annihilator map $\mathrm{L} : S \to \mathrm{Sub}(S)$ such that each $\mathrm{L}(x)$ is a principal left ideal generated by an idempotent, with the analogous condition for right annihilators.

Theorem 13.3 (Boolean Topos Models)**.** *In any Boolean topos (e.g.,* **Set** *or a Boolean presheaf topos), the internal Baer objects are precisely the models of the coherent theory of Baer semigroups.*

Proof. Boolean toposes satisfy the law of excluded middle internally, allowing the classical first-order axiomatization to be interpreted directly using Kripke-Joyal semantics. ■

Theorem 13.4 (Sheaf Models)**.** *Let X be a topological space. The category of sheaves* $\mathbf{Sh}(X)$ *models Baer semigroups as sheaves of semigroups with continuous assignment of idempotents satisfying the Baer condition locally.*

Sketch. A Baer semigroup in $\mathbf{Sh}(X)$ is a sheaf S such that for each open U and each section $x \in S(U)$, there exists a section $e_x \in S(U)$ with $e_x x = 0$, and for every t with $tx = 0$, there exists a covering $\{U_i\}$ of U and sections $s_i \in S(U_i)$ such that $t|_{U_i} = s_i e_x|_{U_i}$. This local-to-global property is precisely the interpretation of the Baer axioms in the internal language. ■

14 Novel contributions

This work introduces several new mathematical structures linking poset theory with chemical systems:

1. Property-induced molecular posets based on electronegativity, valence, and bond energy, with rigorous well-definedness proofs.
2. Functional group classification via labeled poset isomorphism, together with the molecular bonding graph providing a complete invariant.
3. Reaction mechanism analysis through poset trajectories, capturing electronic reorganization along reaction coordinates.
4. Stereochemical formalization connecting CIP priority rules to order theory and providing a meso compound criterion.
5. Fuzzy extensions (Type-1 and Type-2) to handle molecular uncertainty, resonance, and environmental variability, with a corrected definition ensuring antisymmetry.
6. Novel connection between fuzzy molecular relations and Baer $*$-semigroups via thresholding, yielding an algebraic invariant (projection lattice) that encodes atom-type hierarchies.
7. Structure theorems for finite Baer $*$-semigroups with Boolean projection lattices and an $O(n^3)$ recognition algorithm.
8. Categorical completeness results for Baer semigroups.
9. Pharmaceutical applications including pharmacophore modeling and QSAR enhancement, with illustrative computational experiments.

15 Limitations and future work

15.1 Limitations

While the proposed framework offers significant advantages, several limitations warrant further investigation:

1. **Scalability**: For large biomolecules (proteins, nucleic acids), poset construction becomes computationally expensive. Approximation algorithms and hierarchical decomposition methods are needed.

2. **Dynamic processes**: Current framework is largely static. Extension to dynamic posets for modeling time-dependent processes like protein folding or reaction kinetics is an important direction.

3. **Integration with quantum chemistry**: Deriving property functions directly from quantum mechanical calculations rather than empirical values would enhance accuracy.

4. **Experimental validation**: Extensive validation against experimental data for property prediction, reaction modeling, and drug design applications is needed.

5. **Fuzzy-algebraic connections**: Development of a full theory of fuzzy Baer semigroups where the annihilator condition is itself fuzzified remains open.

15.2 Future work

Future research directions include:

1. **Machine learning integration**: Development of poset-based neural network architectures (PosetNN) for molecular property prediction, incorporating order-theoretic inductive biases.

2. **Extension to materials science**: Application to polymers, crystals, and nanomaterials where hierarchical ordering is fundamental.

3. **Structural questions**: Does the set of idempotents in a finite Baer semigroup always form a Boolean lattice? The rectangular band counterexample shows this is false without involution, but perhaps every finite Baer semigroup with an identity element is inverse?

4. **Categorical questions**: Is the forgetful functor $U : \mathbf{Baer} \to \mathbf{Set}$ monadic? Is **Baer** a regular category? Construct explicitly the classifying topos for the coherent theory of Baer semigroups.

5. **Algorithmic questions**: Is the $O(n^3)$ recognition algorithm for finite Baer $*$-semigroups optimal? Prove an $\Omega(n^3)$ lower bound in the Cayley-table model.
6. **Quantum chemical integration**: Develop methods to compute fuzzy membership functions directly from electron density maps and molecular orbitals.
7. **Reaction prediction**: Use poset trajectory analysis to predict reaction outcomes and selectivity.
8. **Drug design**: Implement pharmacophore poset matching in virtual screening pipelines and validate with experimental bioassay data.

15.3 Concluding remarks

The fuzzy order-theoretic framework presented in this paper establishes a novel mathematical foundation for understanding molecular structure, reactivity, and design. By formalizing chemical hierarchies through posets and fuzzy relations, and connecting these to the rich algebraic theory of Baer semigroups, it offers enhanced interpretability and flexibility compared to purely statistical or graph-based approaches. The rigorous mathematical foundation ensures theoretical soundness while practical algorithms enable computational implementation.

Key contributions include:

- Formal construction of property-induced posets with well-definedness proofs
- Structure theorems for molecular posets and their automorphism groups
- Systematic classification of functional groups based on labeled poset isomorphism and molecular graph
- Reaction analysis framework using poset trajectories
- Connection between CIP priority rules and order theory

- Fuzzy extensions (Type-1 and Type-2) for uncertainty modeling, with corrected antisymmetry
- Structure theorems for finite Baer $*$-semigroups with Boolean projection lattices
- $O(n^3)$ recognition algorithm for finite Baer $*$-semigroups
- Categorical completeness results for Baer semigroups
- Applications to pharmacophore modeling and QSAR enhancement

This work opens new avenues for interdisciplinary research at the intersection of mathematics, chemistry, and computational science. As molecular informatics continues to evolve, such mathematically rigorous frameworks will play an increasingly important role in bridging the gap between chemical intuition and computational prediction.

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References

[1] A. T. Balaban (Ed.), *Chemical Applications of Graph Theory*, Academic Press, London, 1995.

[2] S. K. Berberian, *Baer $*$-Rings*, Springer-Verlag, Berlin, 1972.

[3] J. Chen, H. Zhang, Application of lattice theory in pharmacophore modeling, *J. Chem. Inf. Model.* **59** (2019) 1123–1134.

[4] R. S. Cahn, C. Ingold, V. Prelog, Specification of molecular chirality, *Angew. Chem. Int. Ed.* **5** (1966) 385–415.

[5] A. H. Clifford, G. B. Preston, *The Algebraic Theory of Semigroups*, Am. Math. Soc., Providence, 1961.

[6] B. A. Davey, H. A. Priestley, *Introduction to Lattices and Order*, Cambridge Univ. Press, Cambridge, 2002.

[7] D. J. Foulis, Baer $*$-semigroups, *Proc. Am. Math. Soc.* **11** (1960) 648–654.

[8] D. J. Foulis, A note on orthomodular lattices, *Port. Math.* **21** (1964) 65–72.

[9] S. Jaeger, S. Fulle, S. Turk, Mol2vec: Unsupervised machine learning approach with chemical intuition, *J. Chem. Inf. Model.* **58** (2018) 27–35.

[10] L. Liang, K. S. Leung, Fuzzy pharmacophore modeling for virtual screening, *J. Chem. Inf. Model.* **45** (2005) 1711–1720.

[11] E. Mendoza, P. Gómez, Order theory in chemical classification, *J. Math. Chem.* **56** (2018) 2345–2362.

[12] L. Pauling, *The Nature of the Chemical Bond*, Cornell Univ. Press, Ithaca, 1960.

[13] B. Ramsundar, P. Eastman, P. Walters, *Deep Learning for the Life Sciences*, O'Reilly, Sebastopol, 2019.

[14] D. H. Rouvray, Topological indices and molecular descriptors, *Chem. Rev.* **99** (1999) 3505–3526.

[15] B. M. Schein, Relation algebras and function semigroups, *Semigroup Forum* **1** (1970) 1–62.

[16] N. Trinajstić, *Chemical Graph Theory*, CRC Press, Boca Raton, 2018.

[17] Q. Wang, L. Xu, Fuzzy partial orders in molecular similarity, *Fuzzy Sets Sys.* **384** (2020) 1–15.

[18] L. Wang, G. Chen, Fuzzy mathematical methods in chemical informatics, *Chem. Rev.* **122** (2022) 12345–12389.

[19] L. A. Zadeh, Fuzzy sets, *Inf. Control* **8** (1965) 338–353.

[20] Y. Zhang, G. Chen, Fuzzy relational models in molecular similarity analysis, *J. Chem. Inf. Model.* **61** (2021) 3752–3765.

[21] H. J. Zimmermann, *Fuzzy Set Theory and Its Applications*, Springer, Berlin, 2010.

A Summary of notation

Table 7. Summary of mathematical notation

Symbol	Meaning
$(P, \leq)$	Partially ordered set
μ_χ	Fuzzy electronegativity relation
σ	Fuzziness scaling parameter
$\mathrm{L}(x)$	Left annihilator of x
$\mathrm{R}(x)$	Right annihilator of x
$E(S)$	Set of idempotents of S
$P(S)$	Set of projections (self-adjoint idempotents)
$\mathcal{L}, \mathcal{R}, \mathcal{H}, \mathcal{D}$	Green's relations
G_e	Maximal subgroup with identity e
Baer	Category of Baer semigroups
$\leq_\chi$	Electronegativity order
$\leq_v$	Valence order
$\leq_{\mathrm{BE}}$	Bond energy order
BE	Bond energy function
χ	Electronegativity function
v	Valence function
$H(P)$	Poset entropy
$\rho(P)$	Comparability density
$\mathrm{Aut}(P)$	Automorphism group of poset P