

Cage-Constrained Chemical Reachability in π -Stacked Chrysene–Adenosine Systems: Existence, Stereochemical Selection, and Local Transformation Invariance

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Abstract

We develop a mathematical existence theory for constrained chemical transformation in a π -stacked chrysene–adenosine molecular architecture. Starting from a fixed chrysene molecular anchor and a saturated local tether of the form $C6 - O - C_\alpha H_2 - C_\beta H_2 - OPO_3 R_A$, we define persistent-atom typed molecular states, local chemical graph-rewrite rules, cage-admissible configuration spaces, and a free reaction category whose morphisms are finite sequences of chemically admissible, geometrically liftable transformations. An explicit conditional witness reaches the target connectivity $C5 - C_\alpha(H)(NH_2) - C_\beta(=O) - O_2'Ado$ while preserving the inherited chrysene $C5-C6$ carbon-framework bond and complete atom provenance. A separate oriented-cage condition yields stereochemical selection $\chi(c_\alpha) = \chi_\star$.

We prove local transformation invariance across the $\{6, 12\}$, $\{3, 6, 12\}$, and $\{3, 6, 9, 12\}$ substitution contexts. Chemical rewrite transport is exact under local concordance and reaction-inert external context; cage-level persistence additionally requires corresponding candidate geometric lifts whose hard-constraint deviation satisfies $\Delta_{\mathcal{F}}^A < m_{\min}$. Alternative carbonyl factorizations, dual-cipher source–capture transport, and adenine-anchor variants are incorporated without requiring reaction-word or realization uniqueness. The resulting theory establishes conditional target reachability and stereochemically refined existence under explicit hypotheses, while a separate certification framework specifies how those hypotheses may be tested computationally and experimentally.

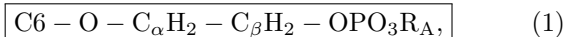
Keywords: chrysene formalism; chemical graph rewriting; molecular cage; chemical reachability; stereochemical selection; local transformation invariance; atom provenance; adenosine; supramolecular chemistry

1 Introduction

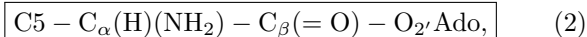
A molecular transformation may be admissible as a change of chemical connectivity while remaining inaccessible in the three-dimensional environment of the molecular system intended to realize it. Conversely, spatial proximity of two reactive groups does not by itself establish a chemically admissible bond transformation. These distinctions are particularly important in constrained supramolecular systems, where tethering, aromatic stacking, stereochemical confinement, and local reaction geometry may restrict the set of transformations available to an embedded molecular state.

The present paper develops a mathematical existence theory for such a problem in a π -stacked chrysene–adenosine architecture. The reference starting motif is the saturated

tether



embedded in an adenosine-bearing cage realization. The target molecular architecture contains



while preserving the inherited chrysene $C5 - C6$ carbon-framework edge.

The mathematical question is not merely whether a sequence of reaction arrows can be written between Equations (1) and (2). It is whether one can construct a well-typed reaction system in which the initial state has at least one finite path to the target while simultaneously preserving persistent atom identity, chemical admissibility, declared cage constraints, and, under stronger hypotheses, a specified stereochemical outcome.

This requires four logically distinct levels:

$$\boxed{\text{molecular connectivity} \neq \text{chemical admissibility} \neq \text{geometric accessibility} \neq \text{physical kinetics.}} \quad (3)$$

The first three are formalized explicitly in the present reaction theory. The fourth belongs to the realization and certification layer. The general boundary between mathematical reachability and physical instantiation is stated in Convention 2.2.

1.1 From typed molecular states to cage-constrained reachability

The molecular framework is built downstream of the inherited Chrysene Formalism. The canonical chrysene molecular anchor, locant registry, primary–dual attachment data, perimeter relation, and directional attachment structure are treated as fixed input. The reaction theory introduced here adds persistent atom identities, chemical state data, local graph-rewrite rules, cage constraints, and stereochemical state information without redefining that molecular foundation.

A chemical state has the form

$$S = (G, \iota, q, r, s, \chi, \rho, \mathcal{K}), \quad (4)$$

where the graph and state labels encode the chemical structure, ρ records reaction resources, and $\mathcal{K}$ records the admissible cage domain.

Local chemical transformations are represented by persistent-atom, typed graph rewrites. These generate the free chemical path category

$$\mathbf{Chem}. \quad (5)$$

A chemically admissible rewrite

$$p : S \longrightarrow S' \quad (6)$$

is promoted to a cage-constrained transition only when it possesses a compatible geometric lift:

$$\text{Lift}_{\mathcal{C}}(p; S, S') \neq \emptyset. \quad (7)$$

The corresponding free reaction category is

$$\boxed{\mathbf{Reach}_{\mathcal{C}}}. \quad (8)$$

Its morphisms are finite ordered words of chemically admissible, cage-liftable elementary transitions.

Accordingly, target existence becomes the categorical statement

$$\text{Hom}_{\mathbf{Reach}_{\mathcal{C}}}(S_0, T) \neq \emptyset. \quad (9)$$

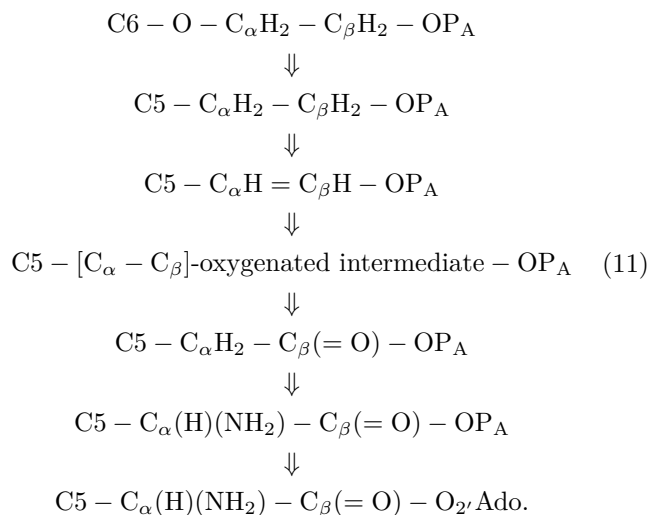
Because $\mathbf{Reach}_{\mathcal{C}}$ is retained as a free category, different reaction rules, matches, or generator orderings remain distinguishable. The theory can therefore separate target existence from reaction-word uniqueness without assigning physical probability to the different words.

1.2 Constructive witness and stereochemical refinement

The existence proof is constructive. For the reference $C6 \rightarrow C5$ architecture, one explicit reaction word is

$$\boxed{\Phi_{\text{can}} = p_{\text{tr}} \circ p_{\text{am}} \circ p_{\text{carb}} \circ p_{\text{epox}} \circ p_{\text{unsat}} \circ p_{\text{cap}}}. \quad (10)$$

At the level of principal local motifs, this word represents



The displayed sequence is a chosen reaction-word factorization. Its individual generators become a cage-constrained witness only under the explicitly stated chemical and geometric realization hypotheses of Sections 8 and 9.

The carbonyl-forming portion of the canonical word is

$$P_{\beta}^{\text{epox}} = p_{\text{carb}} \circ p_{\text{epox}} \circ p_{\text{unsat}}, \quad (12)$$

and an alternative hydroxylation–oxidation factorization

$$P_{\beta}^{\text{hyd}} = q_{\text{ox}} \circ q_{\text{hyd}} \quad (13)$$

is developed separately. Thus the target-existence problem is not formulated as a unique-reaction-word problem.

The stereochemical claim is also separated from connectivity. Formation of the $c_{\alpha} - n_{\alpha}$ bond produces a stereogenic c_{α} center in the target.

An oriented local frame

$$\mathcal{F}_{\alpha} = (e_1, e_2, e_3) \quad (14)$$

and attack scalar

$$\zeta_{\chi} = \langle u_{\text{att}}, e_3 \rangle \quad (15)$$

distinguish the two local approach branches.

A realization-specific map

$$\kappa_{\alpha} : \{-1, +1\} \longrightarrow \{R, S\} \quad (16)$$

converts the selected geometric branch to an absolute configuration after the complete product substituent ordering is fixed.

Under strong cage exclusion of the opposite branch,

$$\chi(c_\alpha) = \chi_\star. \quad (17)$$

Only after the complete product assignment is specified is $\chi_\star$ identified, when appropriate, with the intended L-series configuration χ_L .

1.3 Local transformation invariance and realization families

The reaction of interest is supported near the $C5/C6$ region, whereas the chrysene core may carry additional remote substituents.

The principal substitution family is

$$\mathcal{L} = \{\{6, 12\}, \{3, 6, 12\}, \{3, 6, 9, 12\}\}. \quad (18)$$

The locality theory separates exact chemical context extension from geometric persistence.

At the chemical level, if two realizations agree on the completed local reaction support

$$U_{\text{rxn}} \quad (19)$$

and their external contexts are reaction inert, the same ordered local rewrite word extends exactly.

The cage-level statement requires additional data. Let a selected reference path have uniform positive hard-constraint margin

$$m_{\min} > 0. \quad (20)$$

For another substitution context Λ , suppose corresponding candidate transported lifts have been supplied. Let

$$\Delta_{\mathcal{F}}^\Lambda \quad (21)$$

denote the maximum deviation of their augmented hard-constraint family from the reference path.

The principal persistence criterion is

$$\Delta_{\mathcal{F}}^\Lambda < m_{\min}. \quad (22)$$

Under this inequality, the candidate transports remain cage admissible.

When stereochemical persistence is also required, the transported amino-installation path must satisfy

$$\sup_t \left| \tilde{\zeta}_\chi(t) - \zeta_\chi(t) \right| < \delta_\chi. \quad (23)$$

Thus local transformation invariance means that the same local reaction architecture possesses admissible transported realizations across the declared substitution family.

It does not require the complete molecular geometries to be identical.

The same transport framework also permits other realization changes. The inherited primary–dual locant pairing motivates a

$$C5 \rightarrow C6 \quad (24)$$

dual-cipher architecture, while the reference adenine anchor

$$\eta_A = C2 \quad (25)$$

may be replaced by alternatives such as

$$\eta_A = N6. \quad (26)$$

These variants may preserve the local chemical grammar while changing the cage realization. They are therefore treated as separate realization-indexed reaction categories rather than being identified a priori.

1.4 Principal theorem and certification interface

The main theorem combines the reference constructive witness with the locality and stereochemical transport results.

Under the reference hypothesis package and the family-level locality conditions, for every

$$\Lambda \in \mathcal{L} \quad (27)$$

there exists a complete target state

$$T_\star^\Lambda \in \mathfrak{T}_\star^\Lambda \quad (28)$$

such that

$$\text{Hom}_{\mathbf{Reach}_\Lambda^{6 \rightarrow 5}}(S_0^\Lambda, T_\star^\Lambda) \neq \emptyset, \quad (29)$$

with

$$\chi_{T_\star^\Lambda}(c_\alpha) = \chi_\star. \quad (30)$$

A separate connectivity theorem removes the stereochemical hypothesis and concludes only

$$T_{\text{conn}}^\Lambda \in \mathfrak{T}_{\text{conn}}^\Lambda. \quad (31)$$

Hence

$$\boxed{\text{stereochemically specified reachability} \implies \text{connectivity reachability}} \quad (32)$$

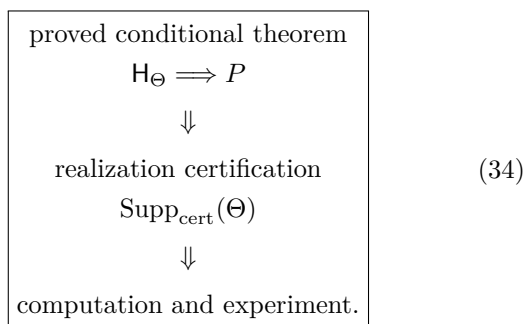
while the converse requires additional stereochemical information.

The theory is paired with a realization-certification architecture

$$G_0, G_1, \dots, G_7, \quad (33)$$

with alternative certification fronts when more than one reaction word is available.

The logical relationship is



This structure permits one reaction route to fail certification without implying failure of target reachability when an independent certified route remains available.

1.5 Organization of the paper

Section 2 specifies the relation between the inherited Chrysene Formalism and the new reaction-realization layer.

Section 3 defines the π -stacked chrysene-adenosine realization family, the saturated reference tether, substitution contexts, initial state, and target architecture.

Section 4 introduces persistent atom identities, typed molecular states, conservation bookkeeping, local reaction rules, and the completed reaction support.

Section 5 defines projected cage domains, geometric liftability, capture and transfer geometry, stereochemical attack regions, and positive constraint margins.

Section 6 constructs **Chem** and **Reach_C** and develops local reaction-category transport.

Section 7 proves exact chemical context extension and the candidate-path persistence theorem underlying substitution invariance.

Section 8 constructs the explicit $C6 \rightarrow C5$ witness.

Section 9 proves the reference and family-level connectivity and stereochemical existence theorems.

Section 10 treats alternative carbonyl factorizations, reaction-word nonuniqueness, dual-cipher transport, adenine-anchor transport, and realization nonuniqueness.

Section 11 defines the logical certification framework.

Sections 12 and 13 interpret and summarize the resulting existence and realization program.

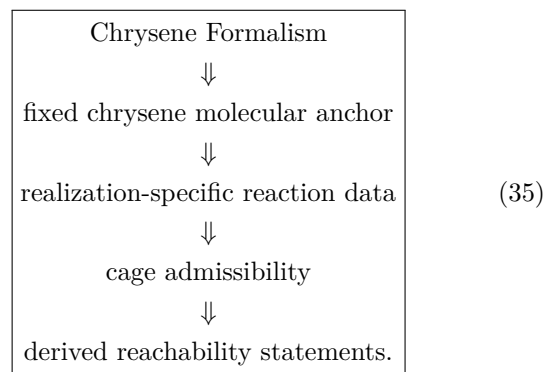
Appendices A–G provide the persistent atom registry, complete local rewrite rules, explicit cage inequalities, technical proofs, secondary path-space and realization-transport results, source and notation concordance, and detailed computational and experimental certification protocols.

2 Relation to the Chrysene Formalism

The present work is a realization-level extension of the Chrysene Formalism rather than a modification of its molecular, tensorial, noncommutative, spectral, or operator-theoretic foundations [?, ?].

The inherited theory supplies the canonical chrysene molecular anchor, locant registry, primary–dual attachment data, perimeter relations, and directional attachment structure. The present paper adds chemical-state, reaction, cage, and stereochemical data over that fixed foundation.

The logical dependence is



2.1 Inherited molecular data

Let

$$\mathcal{C}_{\text{chr}} = (V_{\text{chr}}, E_{\text{chr}}, \iota_{\text{chr}}, \lambda_{\text{chr}}) \quad (36)$$

denote the canonical embedded and labeled chrysene molecular reduct inherited from the foundational theory.

Its carbon-skeleton graph is

$$G_{\text{chr}} = (V_{\text{chr}}, E_{\text{chr}}), \quad (37)$$

with reference embedding

$$\iota_{\text{chr}} : V_{\text{chr}} \longrightarrow \mathbb{R}^3, \quad (38)$$

and inherited label family

$$\lambda_{\text{chr}}. \quad (39)$$

For every distinguished carbon locant j , write

$$v_j \in V_{\text{chr}}, \quad \lambda_{\text{loc}}(v_j) = j. \quad (40)$$

The inherited primary and dual locant sets are

$$\mathcal{S}_{\text{pri}} = \{3, 6, 9, 12\}, \quad \mathcal{S}_{\text{dual}} = \{2, 5, 8, 11\}, \quad (41)$$

with associated vertex sets

$$\begin{aligned} \mathcal{A}_{\text{pri}} &= \{v_3, v_6, v_9, v_{12}\}, \\ \mathcal{A}_{\text{dual}} &= \{v_2, v_5, v_8, v_{11}\}. \end{aligned} \quad (42)$$

The canonical carbon-framework classification is inherited rather than reproved here. A realization may alter substitution, stacking, strain, solvent environment, local bond order, or cage geometry without thereby changing the identity or locant registry of the underlying chrysene carbon framework.

Convention 2.1 (Fixed molecular anchor). Throughout the present paper, $\mathcal{C}_{\text{chr}}$ is fixed.

Reaction-state extensions may modify only those bond, charge, electronic, stereochemical, resource, or geometric data permitted by the declared realization and reaction support. The canonical chrysene carbon-skeleton graph and its inherited locant assignment remain fixed data.

Convention 2.2 (Realization boundary). Unless a stronger conclusion is stated explicitly, a result concerning chemical reachability, cage liftability, reaction-word transport, or stereochemical geometry is interpreted at the corresponding mathematical level.

Claims concerning activation free energies, rate constants, quantum yields, dominant physical mechanism, experimentally populated intermediates, product distributions, or experimental observability require separate realization hypotheses or certification.

Convention 2.2 will be used throughout the paper in place of repeatedly restating the same physical scope qualification.

2.2 Primary–dual cipher and the reactive locant pair

The inherited primary-to-dual locant map is

$$\delta_{\text{dc}} : \mathcal{S}_{\text{pri}} \longrightarrow \mathcal{S}_{\text{dual}}, \quad (43)$$

defined by

$$\begin{aligned} \delta_{\text{dc}}(3) &= 2, & \delta_{\text{dc}}(6) &= 5, \\ \delta_{\text{dc}}(9) &= 8, & \delta_{\text{dc}}(12) &= 11. \end{aligned} \quad (44)$$

Its associated involution on $\mathcal{S}_{\text{pri}} \sqcup \mathcal{S}_{\text{dual}}$ is denoted

$$\sigma_{\text{dc}}, \quad \sigma_{\text{dc}}^2 = \text{id}. \quad (45)$$

The present construction uses principally the paired locants

$$6 \xrightarrow{\delta_{\text{dc}}} 5. \quad (46)$$

The reference source–capture ordering is therefore

$$(6, 5), \quad (47)$$

where $C6$ is the reference tether-bearing site and $C5$ is the adjacent candidate capture site.

The paired alternative considered in Section 10 uses

$$(5, 6). \quad (48)$$

Remark 2.3 (Dual cipher versus molecular symmetry). The map δ_{dc} acts on inherited locant data. It is not assumed to belong to the Euclidean symmetry stabilizer of a chemically instantiated realization. Accordingly, the pairing

$$6 \longleftrightarrow 5$$

supplies a local reaction-support correspondence, not an equality of the two realized cage geometries or physical reaction parameters.

2.3 Perimeter adjacency of the reactive pair

Let

$$\partial G_{\text{chr}} \quad (49)$$

denote the distinguished oriented external perimeter cycle of the canonical chrysene graph.

The inherited perimeter realization of the primary–dual pairing gives the local graph relation required by the reference reaction construction.

Lemma 2.4 (Primary–dual adjacency at $C6/C5$). *The vertices v_6 and v_5 belong to the distinguished external perimeter and are adjacent:*

$$v_6, v_5 \in V(\partial G_{\text{chr}}) \quad (50)$$

and

$$\boxed{\{v_6, v_5\} \in E(\partial G_{\text{chr}})}. \quad (51)$$

Proof. The inherited perimeter-realized dual-cipher condition gives

$$\{v_j, v_{\delta_{\text{dc}}(j)}\} \in E(\partial G_{\text{chr}}) \quad (j \in \mathcal{S}_{\text{pri}}). \quad (52)$$

Taking $j = 6$ and using $\delta_{\text{dc}}(6) = 5$ gives Equation (51). $\square$

Lemma 2.4 supplies graph-theoretic adjacency only. Formation of the new $v_5 - c_\alpha$ bond is represented later by a chemical rewrite, while its spatial accessibility is imposed separately by the cage constraints of Section 5.

2.4 Directional attachment data and local orientation

The inherited formalism equips distinguished attachment vertices with oriented attachment data.

Let

$$\mathbb{S}^2 = \{u \in \mathbb{R}^3 : \|u\|_2 = 1\} \quad (53)$$

and let

$$\tau : \mathcal{A}_{\text{pri}} \longrightarrow \mathbb{S}^2, \quad \tau(v_j) = t_j, \quad (54)$$

denote the inherited outward attachment-tangent map.

For a chemically instantiated tether attached at locant ℓ , let

$$u_{\text{tet}}^{(\ell)} \in \mathbb{S}^2 \quad (55)$$

be its specified local direction.

Define the local orientation scalar

$$\pi_\ell := \left\langle u_{\text{tet}}^{(\ell)}, t_\ell \right\rangle \in [-1, 1]. \quad (56)$$

When only the orientation class is required, define

$$\varepsilon_\ell := \text{sgn}(\pi_\ell) \in \{-1, 0, +1\}. \quad (57)$$

The quantities π_ℓ and ε_ℓ are geometric orientation data. They are not identified by definition with a molecular dipole moment, partial charge, electric polarization, or electrostatic potential.

A realization may replace π_ℓ with a more refined orientation or polarity operator, provided that the replacement is explicitly typed and its transformation law is specified. The reachability theory requires only the relevant geometric datum used by the declared cage constraints.

2.5 Reaction realizations over the foundational theory

Let

$$\mathbf{P}_{\text{CF}} = (\Sigma_{\text{CF}}, \mathbf{T}_{\text{CF}}) \quad (58)$$

denote the inherited formal presentation of the Chrysene Formalism.

Introduce a disjoint collection of realization symbols

$$\Sigma_{\text{rxn}} \quad (59)$$

for chemical states, persistent atom maps, graph rewrites, cage constraints, resource data, stereochemical labels, and realization parameters.

Define the extended signature

$$\Sigma_{\text{ext}} = \Sigma_{\text{CF}} \sqcup \Sigma_{\text{rxn}}. \quad (60)$$

Definition 2.5 (Reaction realization). A *reaction realization* is a Σ_{ext} -structure $\mathcal{R}$ such that:

1. its reduct to the inherited signature satisfies

$$\text{Red}_{\Sigma_{\text{CF}}}(\mathcal{R}) \models \mathbf{T}_{\text{CF}}; \quad (61)$$

2. its molecular reduct contains the fixed anchor $\mathcal{C}_{\text{chr}}$ of Convention 2.1; and

3. all additional chemical and geometric data are supplied through explicitly declared realization structures and hypotheses.

Let

$$\mathbf{H}_{\text{rxn}} \quad (62)$$

denote the realization-specific chemical, cage, resource, and stereochemical hypotheses used by a selected construction.

Let

$$\mathbf{T}_{\text{reach}} \quad (63)$$

denote the definitions and mathematical rules governing chemical and cage-constrained state transformations.

The realization-level extension may therefore be written

$$\mathbf{T}_{\text{ext}} = \mathbf{T}_{\text{CF}} \cup \mathbf{H}_{\text{rxn}} \cup \mathbf{T}_{\text{reach}}. \quad (64)$$

No specific bond-breaking, bond-forming, oxidation, amination, stereochemical-selection, or acyl-transfer rule is inherited merely from membership in $\mathbf{T}_{\text{CF}}$. Such transformations enter through $\mathbf{H}_{\text{rxn}}$ and the reaction grammar developed in the present paper.

2.6 Reference and alternative realization parameters

The principal realization uses the ordered source-capture pair

$$C6 \longrightarrow C5. \quad (65)$$

Denote this realization class by

$$\mathcal{R}_{6 \rightarrow 5}. \quad (66)$$

The dual-cipher alternative is

$$\mathcal{R}_{5 \rightarrow 6}, \quad (67)$$

in which the local source and capture roles are exchanged.

A second realization parameter records the adenine-side attachment site:

$$\eta_A \in \{C2, N6, \dots\}. \quad (68)$$

The reference architecture uses

$$\eta_A = C2. \quad (69)$$

Alternative choices, including

$$\eta_A = N6, \quad (70)$$

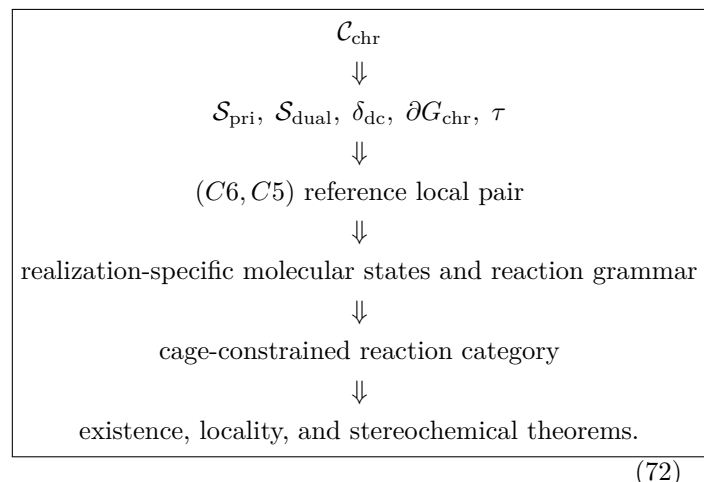
change realization data without altering the fixed chrysene molecular anchor.

A third realization parameter is the remote substitution context Λ , introduced explicitly in Section 3. These realization parameters are later separated into:

- chemical-support changes,
- cage-geometry changes, (71)
- and transported target data.

2.7 Dependency of the present construction

The inherited and newly constructed parts of the paper can now be displayed as



The first two levels are inherited from the foundational theory. The remaining levels are constructed in the present work.

Section 3 now specifies the molecular realization family on which those new reaction and cage structures act.

3 The π -Stacked Chrysene–Adenosine Realization Class

We now specify the molecular realization family on which the reaction and cage constructions of the following sections act.

These objects are realization data over the fixed chrysene molecular anchor of Section 2; they are not additional axioms of the inherited Chrysene Formalism.

The reference architecture contains four structural ingredients:

1. a substituted chrysene realization containing the inherited $C5/C6$ perimeter pair;
2. a saturated two-carbon oxygenated tether initially attached through $C6$;
3. a phosphate-containing connection to an adenosine-bearing component; and
4. an embedded local cage in which the chrysene and adenine aromatic systems satisfy explicitly declared π -stack constraints.

Related substituted-chrysene, stacked, nucleoside-linked, and spatially constrained molecular architectures provide motivating realization classes. Their use here is structural; all chemical and physical claims remain subject to Convention 2.2.

3.1 Substitution contexts

Define

$$\mathcal{L} = \{\Lambda_2, \Lambda_3, \Lambda_4\} \quad (73)$$

with

$$\Lambda_2 = \{6, 12\}, \quad \Lambda_3 = \{3, 6, 12\}, \quad \Lambda_4 = \{3, 6, 9, 12\}. \quad (74)$$

For $\Lambda \in \mathcal{L}$, let

$$C^\Lambda \quad (75)$$

denote a chemically decorated realization of the fixed chrysene carbon-skeleton graph G_{chr} whose substituted locants include those recorded by Λ .

The index Λ records substitution context only. It does not require all substituents to be chemically identical and does not imply equality of their three-dimensional local environments.

The $C6$ site is distinguished in the reference realization as the initial tether-bearing site. The remaining substituted positions are treated as external context unless they enter a subsequently declared reaction-rule pattern.

This separation allows the local transformation problem to be posed independently of the number of additional remote chrysene substitutions.

3.2 Reference tether and adenosine-bearing domain

Introduce persistent non-chrysene carbon atoms

$$c_\alpha, \quad c_\beta, \quad (76)$$

where c_α is proximal and c_β is distal relative to the reference $C6$ attachment.

Let

$$o_6 \quad (77)$$

denote the oxygen initially connecting v_6 to c_α , and let

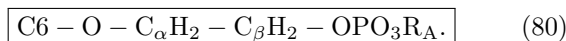
$$o_\beta \quad (78)$$

denote the oxygen connecting c_β to the phosphate-containing domain.

The reference local connectivity is

$$v_6 - o_6 - c_\alpha - c_\beta - o_\beta - P_A, \quad (79)$$

represented schematically as



Equation (80) specifies connectivity rather than a complete phosphate protonation or counterion state. Formal charge and resource bookkeeping are introduced in Section 4.

The initial $c_\alpha - c_\beta$ bond is saturated:

$$\bar{b}(c_\alpha, c_\beta) = 1. \quad (81)$$

Unsaturated and oxidized forms are intermediate-state data rather than part of the reference starting architecture.

Let

$$A_{\text{Ado}} \quad (82)$$

denote a labeled adenosine molecular graph containing an adenine base and ribofuranose unit.

Distinguish the adenine $C2$ site

$$a_2, \quad \lambda_A(a_2) = C2, \quad (83)$$

and the persistent ribose oxygen

$$o_{2'} \quad (84)$$

belonging initially to the free $2'$ -hydroxyl group.

Definition 3.1 (Adenine anchor parameter). Let

$$\eta_A \quad (85)$$

denote the selected adenine-side tether attachment site. The reference realization uses

$$\boxed{\eta_A = C2.} \quad (86)$$

Alternative realizations may use

$$\eta_A = N6 \quad (87)$$

or another explicitly defined attachment site.

Let

$$L_A \quad (88)$$

be the finite labeled linker graph connecting the phosphate domain to the selected adenine-side anchor.

Write the phosphate-containing adenosine-side domain abstractly as

$$P_A = P(L_A, A_{\text{Ado}}, \eta_A). \quad (89)$$

Its internal realization may vary provided every atom entering the chemical reaction support or geometric cage support is represented explicitly.

Before terminal acyl transfer, the persistent ribose oxygen $o_{2'}$ is not bonded to the eventual acyl carbon:

$$\bar{b}(c_\beta, o_{2'}) = 0. \quad (90)$$

3.3 The local π -stacked cage cell

The reference realization is embedded in a local supramolecular cage rather than treated as an unconstrained molecular graph.

Let

$$\Pi_{\text{chr}}, \quad \Pi_A \quad (91)$$

denote reference least-squares planes for the chrysene and adenine aromatic frameworks whenever they are well defined for the selected configuration.

Choose unit normals

$$n_{\text{chr}}, n_A \in \mathbb{S}^2. \quad (92)$$

Define the interplanar alignment observable

$$\Theta_\pi := \arccos(|\langle n_{\text{chr}}, n_A \rangle|) \in \left[0, \frac{\pi}{2}\right]. \quad (93)$$

Let

$$c_{\text{chr}}, \quad c_A \quad (94)$$

denote the corresponding aromatic centroids.

Define the normal stack separation

$$d_\pi := |\langle c_A - c_{\text{chr}}, n_{\text{chr}} \rangle|, \quad (95)$$

and the in-plane displacement

$$s_\pi := \|(I - n_{\text{chr}} n_{\text{chr}}^\top)(c_A - c_{\text{chr}})\|_2. \quad (96)$$

Definition 3.2 (π -stack admissibility window). A local cage configuration is π -stack admissible when

$$d_\pi \in I_d, \quad s_\pi \in I_s, \quad \Theta_\pi \in I_\theta, \quad (97)$$

for prospectively specified compact intervals

$$I_d, \quad I_s, \quad I_\theta. \quad (98)$$

These quantities define geometric stacking observables. The complete cage-admissible configuration space and transition constraints are defined in Section 5.

Remark 3.3 (Optional repeated-stack extension). A larger realization may contain a finite or repeated family of local cage cells

$$\{\mathfrak{c}_k^\Lambda\}_{k \in I}, \quad I \subseteq \mathbb{Z}, \quad (99)$$

with registry data specifying relative translation and orientation of neighboring cells.

No theorem in the present paper requires an infinite stack, periodicity, a thermodynamic limit, or long-range electronic coherence. Only the finite cage neighborhood entering the declared reaction constraints is required.

3.4 Reference initial realization

For each

$$\Lambda \in \mathcal{L}, \quad (100)$$

denote the reference initial molecular state by

$$S_0^\Lambda. \quad (101)$$

Its local reactive subgraph contains

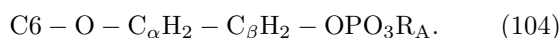
$$v_6 - o_6 - c_\alpha - c_\beta - o_\beta - P_A, \quad (102)$$

with

$$\bar{b}(c_\alpha, c_\beta) = 1 \quad (103)$$

and unacylated $o_{2'}$.

The corresponding schematic local structure is



The state S_0^Λ also carries the realization-specific charge, electronic, stereochemical, resource, reference-embedding, and cage data required by the formal state definition of Section 4.

Thus two realizations may have the same local molecular connectivity while representing distinct states because their charge, resources, electronic labels, reference embedding, or admissible cage domains differ.

3.5 Principal target connectivity and stereochemistry

The principal target contains a new carbon-carbon bond between the persistent tether carbon c_α and the chrysene $C5$ vertex.

Let

$$G_\star^{\text{main}} \quad (105)$$

denote the principal persistent-atom-labeled target graph.

Its local connectivity requires

$$v_5 - c_\alpha - c_\beta - o_{2'}, \quad (106)$$

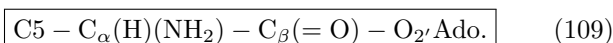
together with

$$\bar{b}(c_\beta, o_{\text{carbonyl}}) = 2 \quad (107)$$

and an amino substituent

$$\bar{b}(c_\alpha, n_\alpha) = 1. \quad (108)$$

Schematically,



The inherited chrysene carbon-framework bond is preserved:

$$\bar{b}_{G_\star}(v_5, v_6) = \bar{b}_{G_{\text{chr}}}(v_5, v_6). \quad (110)$$

Thus target formation does not include opening of the inherited $C5 - C6$ chrysene edge.

Definition 3.4 (Target stereochemical label). Let

$$\chi_\star \in \{R, S\} \quad (111)$$

denote the desired absolute configuration at c_α after the complete product substituent-priority ordering has been specified.

When the realized product configuration corresponds to the intended L-series assignment under the applicable biochemical convention, write

$$\chi_\star = \chi_L. \quad (112)$$

No universal identification $\chi_L = R$ or $\chi_L = S$ is assumed.

3.6 Complete terminal states and coproduct bookkeeping

The principal product does not, by itself, contain every persistent atom in the closed reaction universe.

Let

$$\mathcal{Z}_6 \quad (113)$$

denote the declared class of admissible terminal states containing the original tether oxygen o_6 .

Let

$$\mathcal{Z}_P \quad (114)$$

denote the corresponding class for the departing phosphate-containing fragment, and let

$$\mathcal{Z}_H \quad (115)$$

denote allowed terminal or intermediate states of mapped hydrogens transferred from the principal molecular component.

Definition 3.5 (Complete target realization). A complete terminal realization T^Λ is a target realization when:

1. its principal-product projection contains $G_\star^{\text{main}}$;
2. when stereochemistry is included in the target,

$$\chi_{T^\Lambda}(c_\alpha) = \chi_\star;$$

3. o_6 belongs to an allowed member of $\mathcal{Z}_6$;
4. the departing phosphate-containing fragment belongs to an allowed member of $\mathcal{Z}_P$;
5. mapped hydrogens outside the principal product belong to allowed members of $\mathcal{Z}_H$; and
6. every persistent atom in the closed reaction universe occurs exactly once in the complete terminal state.

Define the principal-product projection

$$\pi_{\text{main}}(T^\Lambda) \quad (116)$$

by forgetting coproduct components not belonging to the principal product while retaining the persistent target atom identities.

The connectivity and stereochemical target classes used in the main existence theorem are formalized in Section 9.

3.7 Structural reaction neighborhood and cage support

Before the reaction grammar itself is defined, isolate the structural neighborhood containing the principal $C5/C6$ -centered transformation.

Define

$$U_6 \subseteq \mathbb{A} \quad (117)$$

to contain at least

$$\boxed{\{v_5, v_6, o_6, c_\alpha, c_\beta, o_\beta, p, o_{2'}\}}. \quad (118)$$

The set U_6 is a *structural reaction neighborhood*. It is not yet the complete rule support.

After the reaction grammar is specified, Section 4 enlarges it to the completed reaction support

$$U_{\text{rxn}} = U_6 \cup \bigcup_{p \in \mathcal{P}_6} \text{Pat}(p), \quad (119)$$

so that every atom inspected by a selected local rule is included.

The geometric cage support may be larger still:

$$\boxed{U_6 \subseteq U_{\text{rxn}} \subseteq C(S)}. \quad (120)$$

Consequently,

$$\text{chemical reaction support} \neq \text{cage support}. \quad (121)$$

An atom may constrain an admissible molecular geometry without undergoing any chemical rewrite.

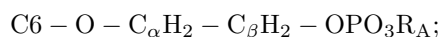
3.8 Reference and alternative realization classes

For $\Lambda \in \mathcal{L}$, define the reference realization class

$$\mathcal{R}_{\Lambda, C2}^{6 \rightarrow 5} \quad (122)$$

to consist of realizations satisfying:

1. the fixed chrysene molecular anchor;
2. substitution context Λ ;
3. the saturated initial tether



4. adenine anchor

$$\eta_A = C2;$$

5. a free 2'-oxygen before terminal transfer;
6. a nonempty declared initial cage domain; and
7. source-capture ordering

$$C6 \longrightarrow C5.$$

Two principal alternative realization families will be considered later.

The dual-cipher family is

$$\mathcal{R}_{\Lambda, C2}^{5 \rightarrow 6}, \quad (123)$$

in which the source and capture locants are exchanged.

The anchor-variant family is

$$\mathcal{R}_{\Lambda, \eta_A}^{6 \rightarrow 5}, \quad \eta_A \neq C2, \quad (124)$$

including the explicitly modeled $N6$ -anchored case.

Neither alternative is assumed to have the same cage geometry or physical reaction parameters as the reference realization.

A convenient realization index is therefore

$$\mathbf{p} = (\Lambda, \eta_A, \ell_{\text{source}}, \ell_{\text{capture}}, \pi_\ell, I_d, I_s, I_\theta, \dots), \quad (125)$$

where additional charge, electronic, resource, and cage parameters are supplied as required by the formal state theory.

The principal stereochemically specified local invariant is

$$\boxed{\mathcal{I}_\star = [v_5 - c_\alpha(H)(NH_2) - c_\beta(=O) - o_{2'}]_{\chi_\star}}. \quad (126)$$

3.9 The reachability problem

The realization family above determines the molecular endpoints of the main mathematical problem.

Problem 3.6 (Cage-constrained chemical reachability). For each

$$\Lambda \in \mathcal{L}, \quad (127)$$

determine explicit sufficient conditions under which there exists a finite atom-map-preserving sequence

$$S_0^\Lambda = S_0 \longrightarrow S_1 \longrightarrow \dots \longrightarrow S_m = T^\Lambda \quad (128)$$

such that:

1. every elementary transformation is chemically admissible;
2. every required elementary transformation admits a compatible cage lift;
3. the protected chrysene framework and persistent atom identities are preserved;

4. the terminal principal-product projection contains $G_{\star}^{\text{main}}$;
5. when stereochemical reachability is asserted,

$$\chi_{T^{\Lambda}}(c_{\alpha}) = \chi_{\star};$$

and

6. the result transports across the declared substitution contexts whenever the chemical and geometric locality hypotheses are satisfied.

Problem 3.6 asks initially for existence of at least one admissible path. Distinct reaction words and alternative molecular realizations are treated separately in Section 10.

The molecular architecture defined in this section supplies the source, target, and realization parameters for that problem. Whether a particular molecular system instantiates the required chemical, cage, stereochemical, or kinetic conditions is governed by Convention 2.2 and the certification framework of Section 11.

The next section replaces these molecular descriptions by formally typed persistent-atom graphs and defines the local reaction grammar used throughout the remainder of the paper.

4 Typed Molecular Graphs and Local Chemical Transformations

The molecular architectures introduced in Section 3 are now represented by finite typed graph objects on which local chemical transformations can be defined exactly.

The present section treats the chemical layer of the theory:

$$\text{persistent atoms} \longrightarrow \text{typed molecular states} \longrightarrow \text{local chemical transformations} \quad (129)$$

Geometric cage admissibility is introduced in Section 5. Thus a chemically admissible rewrite need not yet be geometrically liftable.

4.1 Persistent atom universe and elemental typing

Fix a finite reaction instance and let

$$\mathbb{A} \quad (130)$$

be its finite *persistent atom universe*.

The elements of $\mathbb{A}$ are individual atom identities rather than element symbols. For example,

$$v_5, v_6, o_6, c_{\alpha}, c_{\beta}, o_{\beta}, p, o_{2'} \in \mathbb{A} \quad (131)$$

denote atoms whose identities remain fixed throughout the reaction sequence.

Let

$$\mathcal{E} = \{\text{H, C, N, O, P, } \dots\} \quad (132)$$

be the set of chemical elements used in the realization.

Definition 4.1 (Element map). The *element map* is

$$\epsilon : \mathbb{A} \longrightarrow \mathcal{E}, \quad (133)$$

assigning to each persistent atom identity its chemical element.

The element map is invariant under every reaction transformation:

$$\epsilon_{i+1}(a) = \epsilon_i(a) \quad (a \in \mathbb{A}). \quad (134)$$

When isotopic provenance is required, introduce

$$\mu : \mathbb{A} \longrightarrow \mathbb{N} \quad (135)$$

as an isotopic mass-number map. The map μ is likewise invariant under reaction.

4.2 Typed molecular graphs and persistent molecular labels

Let

$$\mathcal{B} = \{1, 2, 3, \text{ar}\} \quad (136)$$

denote the set of allowed nonzero bond labels.

Definition 4.2 (Typed molecular graph). A *typed molecular graph* is a tuple

$$G = (V, E, \epsilon, b, \lambda) \quad (137)$$

such that:

1. $V \subseteq \mathbb{A}$ is a finite atom set;
- 2.

$$E \subseteq \{\{u, v\} : u, v \in V, u \neq v\}$$

is a finite undirected edge set;

- 3.

$$\epsilon|_V : V \longrightarrow \mathcal{E}$$

is the inherited elemental typing;

- 4.

$$b : E \longrightarrow \mathcal{B}$$

assigns a bond label to every edge; and

5. λ is a finite family of additional partial labels, including locant, molecular-role, cage-role, and persistent atom-role labels whenever required.

Extend the bond map to all unordered atom pairs by

$$\bar{b}_G(u, v) = \begin{cases} b(\{u, v\}), & \{u, v\} \in E, \\ 0, & \{u, v\} \notin E. \end{cases} \quad (138)$$

A bond transformation can therefore be written uniformly as

$$\bar{b}_G(u, v) \mapsto \bar{b}_H(u, v). \quad (139)$$

The inherited chrysene locant map is

$$\lambda_{\text{loc}} : V \rightarrow \mathbb{N}, \quad (140)$$

with

$$\lambda_{\text{loc}}(v_5) = 5, \quad \lambda_{\text{loc}}(v_6) = 6. \quad (141)$$

The tether atoms carry persistent role labels:

$$\lambda_{\text{role}}(c_\alpha) = C_\alpha, \quad \lambda_{\text{role}}(c_\beta) = C_\beta, \quad (142)$$

and

$$\lambda_{\text{role}}(o_6) = O_6, \quad \lambda_{\text{role}}(o_\beta) = O_\beta, \quad \lambda_{\text{role}}(o_{2'}) = O_{2'}. \quad (143)$$

Thus c_β , for example, denotes the same persistent carbon atom before and after carbonyl formation.

4.3 Charge, radical, and electronic-state data

Let

$$q : V \rightarrow \mathbb{Z} \quad (144)$$

be the formal-charge map.

Let

$$r : V \rightarrow \mathbb{N}_0 \quad (145)$$

record explicitly represented localized unpaired electrons.

Global or delocalized electronic-state information is represented by

$$s \in \mathcal{S}_{\text{el}}, \quad (146)$$

where $\mathcal{S}_{\text{el}}$ is a realization-specific set of electronic-state labels.

When a valence rule requires atom-local electronic typing, let

$$\sigma_S(v) \quad (147)$$

denote the local electronic-state label derived from, or supplied in addition to, (q, r, s) .

Remark 4.3 (Formal electronic representation). The data (q, r, s) are formal state labels. They need not coincide with quantum-mechanical partial charges, spin densities, or an exact electronic wavefunction. A physical realization may refine these labels without altering the graph-theoretic definitions below.

4.4 Typed stereochemical state data

Stereochemical labels of tetrahedral atoms and stereogenic bonds have different types and are therefore represented separately.

Define

$$\mathcal{X}_V = \{R, S, \perp\}, \quad (148)$$

and

$$\mathcal{X}_E = \{E, Z, \perp\}, \quad (149)$$

where $\perp$ denotes “not stereochemically assigned in the present state.”

Let

$$\chi_V : V \rightarrow \mathcal{X}_V \quad (150)$$

and

$$\chi_E : E \rightarrow \mathcal{X}_E \quad (151)$$

be the corresponding partial maps.

Any additional axial, helical, or realization-specific stereochemical data may be recorded by a separate partial label family

$$\chi_{\text{aux}}. \quad (152)$$

Write

$$\chi := (\chi_V, \chi_E, \chi_{\text{aux}}) \quad (153)$$

for the complete stereochemical datum.

When no ambiguity can arise, the abbreviation

$$\chi(c_\alpha) := \chi_V(c_\alpha) \quad (154)$$

will be used.

Initially one may have

$$\chi(c_\alpha) = \perp, \quad (155)$$

and at a later state

$$\chi(c_\alpha) = \chi_\star, \quad \chi_\star \in \{R, S\}. \quad (156)$$

Definition 4.4 (Stereochemical refinement). A transformation

$$S \rightarrow S' \quad (157)$$

is a *stereochemical refinement at v* when

$$\chi_V^S(v) = \perp \quad (158)$$

and

$$\chi_V^{S'}(v) \in \{R, S\}, \quad (159)$$

while the persistent atom identity v is preserved.

4.5 Chemical graph admissibility

Because charged atoms, radicals, phosphorus-containing groups, and resonance-stabilized structures may occur, chemical admissibility is not encoded by one universal integer-valence rule.

For each element $Z \in \mathcal{E}$, formal charge $q \in \mathbb{Z}$, and local electronic label σ , let

$$\mathcal{V}_{Z,q,\sigma} \quad (160)$$

be a prospectively specified set of admissible local bond configurations.

For $v \in V$, define the local bond multiset

$$\text{Bond}_G(v) := \{\bar{b}_G(v, u) : u \in V, \bar{b}_G(v, u) \neq 0\}. \quad (161)$$

Definition 4.5 (Locally valence-admissible atom). An atom $v \in V$ is *locally valence admissible* when

$$\text{Bond}_G(v) \in \mathcal{V}_{\epsilon(v), q(v), \sigma_S(v)}. \quad (162)$$

Definition 4.6 (Chemically graph-admissible state). A molecular state is *chemically graph admissible* when every atom is locally valence admissible and every additional declared chemical-graph constraint is satisfied. We write

$$\text{Chem}(G, q, r, s, \chi, \lambda) = 1. \quad (163)$$

Otherwise

$$\text{Chem}(G, q, r, s, \chi, \lambda) = 0. \quad (164)$$

The predicate *Chem* contains chemical graph conditions only. Cage geometry, activation barriers, and kinetic accessibility are not encoded in this predicate.

4.6 Chemical state objects and reference embeddings

Definition 4.7 (Chemical state). A *chemical state* is a tuple

$$S = (G, \iota, q, r, s, \chi, \rho, \mathcal{K}), \quad (165)$$

where:

1. G is a typed molecular graph;
- 2.

$$\iota : V(G) \longrightarrow \mathbb{R}^3$$

is a designated *reference embedding*;

3. q is the formal-charge map;
4. r is the localized radical map;
5. s is the declared electronic-state datum;
6. χ is the typed stereochemical datum;
7. ρ is the reaction-resource ledger; and

8. $\mathcal{K}$ is the associated admissible cage-configuration set defined in Section 5.

The reference embedding ι provides coordinates for molecular registration, initialization, or comparison. It is not, by definition, asserted to belong to $\mathcal{K}(S)$. A realized admissible conformation is represented separately by

$$x \in \mathcal{K}(S). \quad (166)$$

The chemical projection is

$$\pi_{\text{chem}}(S) = (G, q, r, s, \chi, \rho). \quad (167)$$

4.7 Closed reaction universe and conservation bookkeeping

A complete reaction path is evaluated inside a fixed closed reaction universe

$$\Omega_{\text{rxn}}, \quad (168)$$

containing:

1. the initial chrysene–adenosine architecture;
2. all explicitly represented reagent atoms;
3. all atoms that may enter intermediates or products;
4. all explicitly represented coproduct atoms; and
5. any declared nonmolecular excitation, electron, or reservoir bookkeeping data.

For a closed reaction instance,

$$V(S_i) = \mathbb{A} \quad (0 \leq i \leq m), \quad (169)$$

although the graph may contain several connected components.

Consequently, atoms are never created or destroyed by a rewrite.

Lemma 4.8 (Elemental conservation). *Suppose every state in a reaction sequence has the fixed atom universe $\mathbb{A}$ and invariant element map ϵ . Then for every $Z \in \mathcal{E}$,*

$$N_Z(S_i) := \#\{a \in \mathbb{A} : \epsilon(a) = Z\} \quad (170)$$

is independent of i .

Proof. The fiber $\epsilon^{-1}(Z)$ is fixed throughout the sequence. $\square$

4.8 Resource ledger and global charge balance

Let

$$\mathcal{R} \quad (171)$$

be an abelian resource group generated by declared reaction resources, for example

$$\mathcal{R} = \mathbb{Z}\langle H^+, e^-, h\nu, R_1, R_2, \dots \rangle. \quad (172)$$

Atomic reagents represented by vertices of $\mathbb{A}$ remain subject to atom mapping. The ledger ρ does not replace atomic bookkeeping.

Let

$$\mathcal{R}_{\text{adm}} \subseteq \mathcal{R} \quad (173)$$

be the prospectively specified set of allowed resource states.

A state satisfies

$$\rho(S) \in \mathcal{R}_{\text{adm}}. \quad (174)$$

A rule p carries a resource increment

$$\Delta\rho_p \in \mathcal{R} \quad (175)$$

and acts by

$$\rho(S') = \rho(S) + \Delta\rho_p. \quad (176)$$

For example,

$$\Delta\rho_p = -h\nu \quad (177)$$

may encode consumption of one excitation resource.

Let

$$Q_{\text{res}} : \mathcal{R} \longrightarrow \mathbb{Z} \quad (178)$$

be an additive resource-charge map.

A resource represented simultaneously as an explicit molecular component and by a ledger label is counted in only one charge bookkeeping channel.

Define the molecular formal charge

$$Q_{\text{mol}}(S) := \sum_{v \in \mathbb{A}} q_S(v), \quad (179)$$

and the complete charge-bookkeeping quantity

$$Q_{\text{tot}}(S) := Q_{\text{mol}}(S) + Q_{\text{res}}(\rho(S)). \quad (180)$$

Definition 4.9 (Charge-balanced rule application). A rule application

$$S \xRightarrow[p]{} S' \quad (181)$$

is *charge balanced* when

$$Q_{\text{mol}}(S') - Q_{\text{mol}}(S) + Q_{\text{res}}(\Delta\rho_p) = 0. \quad (182)$$

Lemma 4.10 (Global charge conservation). *If every rule application in a finite reaction path is charge balanced, then*

$$Q_{\text{tot}}(S_i) = Q_{\text{tot}}(S_0) \quad (0 \leq i \leq m). \quad (183)$$

Proof. Using Equation (176),

$$Q_{\text{tot}}(S') - Q_{\text{tot}}(S) = Q_{\text{mol}}(S') - Q_{\text{mol}}(S) \quad (184)$$

$$+ Q_{\text{res}}(\Delta\rho_p) \quad (185)$$

$$= 0. \quad (186)$$

Finite induction gives the result. $\square$

Additional additive conservation ledgers, such as an explicitly declared electron-equivalent or redox reservoir, may be incorporated by the same construction.

Remark 4.11 (Excitation bookkeeping). A label such as $h\nu$ is a resource datum rather than an atom identity. Its presence records a condition on a reaction rule; it does not alter the elemental conservation law.

4.9 Local support of a state transformation

Let

$$U \subseteq \mathbb{A}. \quad (187)$$

For a graph G , let

$$G[U] \quad (188)$$

denote the labeled subgraph induced by U .

Definition 4.12 (Bond-change support). For molecular graphs G and H on the same atom universe, define

$$\text{supp}_E(G, H) \quad (189)$$

as the set of atoms incident to at least one pair $\{u, v\}$ for which

$$\bar{b}_G(u, v) \neq \bar{b}_H(u, v). \quad (190)$$

For full states S, S' , define

$$\text{supp}(S, S') = \text{supp}_E(G, G') \cup \text{supp}_q \cup \text{supp}_r \cup \text{supp}_{\chi_V} \cup \text{supp}_{\chi_E}. \quad (191)$$

The global state label s and resource ledger ρ are rule metadata and do not themselves enlarge the atom support.

Definition 4.13 (U -local transformation). A state transformation

$$S \longrightarrow S' \quad (192)$$

is U -local when

$$\text{supp}(S, S') \subseteq U. \quad (193)$$

4.10 Local bond-rewrite rules

Definition 4.14 (Local bond-rewrite rule). A *local bond-rewrite rule* is a tuple

$$p = (L, K, R, \Delta q, \Delta r, \Delta \chi, \Delta \rho), \quad (194)$$

where:

1. L is the labeled reactant pattern;
2. R is the labeled product pattern;
3. K is their preserved labeled interface;
4. Δq , Δr , and $\Delta \chi$ record local state-label changes; and
5. $\Delta \rho$ records resource consumption or production.

At the graph level,

$$L \xleftarrow{\ell} K \xrightarrow{r} R \quad (195)$$

is represented by injective type- and label-preserving maps.

Remark 4.15 (DPO interpretation). The span (195) may be interpreted in a category of finite typed, edge-labeled molecular graphs using the standard double-pushout rewriting construction. For the principal rule family considered here, persistent atom vertices are retained; bond deletion, insertion, and bond-label change supply the principal graph operations.

Define the *pattern support*

$$\text{Pat}(p) := V(L) \cup V(R), \quad (196)$$

under the persistent atom identification supplied by the interface.

Define the *active atom set*

$$\text{Act}(p) \subseteq \text{Pat}(p) \quad (197)$$

as the atoms incident to a changed bond or carrying a changed formal-charge, radical, or stereochemical label.

Thus

$$\text{Act}(p) \subseteq \text{Pat}(p), \quad (198)$$

with strict inclusion possible when unchanged neighboring atoms are required for pattern matching.

4.11 Rule matches and chemical rule application

Definition 4.16 (Rule match). A *match* of p in a molecular graph G is an injective, element-preserving, label-compatible graph map

$$m : L \hookrightarrow G. \quad (199)$$

Persistent atom labels must be preserved whenever they occur in the pattern.

Given a match, write

$$G \xRightarrow[p,m]{} H \quad (200)$$

for the graph-level rewrite and

$$S \xRightarrow[p,m]{} S' \quad (201)$$

for the corresponding state transformation.

Definition 4.17 (Chemically admissible rewrite). A rewrite

$$S \xRightarrow[p,m]{} S' \quad (202)$$

is *chemically admissible* when:

1. the match m preserves all required types and labels;

- 2.

$$\text{Chem}(G', q', r', s', \chi', \lambda') = 1;$$

3. persistent atom identity, element type, and isotope labels are preserved;

- 4.

$$\rho(S') = \rho(S) + \Delta \rho_p \in \mathcal{R}_{\text{adm}};$$

5. the application is charge balanced in the sense of Definition 4.9;

6. every new stereochemical assignment is well typed in the product state; and

7. every declared protected chemical invariant applicable to the rule is preserved.

We write

$$S \xRightarrow[p]{\text{chem}} S' \quad (203)$$

when at least one chemically admissible match exists.

4.12 Reaction grammar and completed local support

Let

$$\mathcal{P} = \{p_\gamma\}_{\gamma \in \Gamma} \quad (204)$$

be the declared reaction grammar.

The rule index set Γ need not correspond one-to-one with named microscopic mechanisms.

For the reference $C6 \rightarrow C5$ construction, let

$$\mathcal{P}_6 \subseteq \mathcal{P} \quad (205)$$

be the selected local rule family.

Let

$$U_6 \supseteq \{v_5, v_6, o_6, c_\alpha, c_\beta, o_\beta, p, o_{2'}\} \quad (206)$$

denote the structural $C5/C6$ -centered support introduced in Section 3.7.

Definition 4.18 (Completed local reaction support).

The *completed local reaction support* of $\mathcal{P}_6$ is

$$U_{\text{rxn}} := U_6 \cup \bigcup_{p \in \mathcal{P}_6} \text{Pat}(p). \quad (207)$$

Consequently,

$$\text{Act}(p) \subseteq \text{Pat}(p) \subseteq U_{\text{rxn}} \quad (p \in \mathcal{P}_6). \quad (208)$$

The use of $\text{Pat}(p)$ rather than only $\text{Act}(p)$ ensures that every atom required to match a selected local rule is contained in the completed support.

For the canonical construction, the grammar may contain generators with the schematic roles

$$\begin{array}{cccc} p_{\text{cap}}, & p_{\text{unsat}}, & p_{\text{ox}}, & p_{\text{carb}}, \\ & p_{\text{am}}, & p_{\text{tr}}. & \end{array} \quad (209)$$

Their exact balanced rule data are specified when the constructive witness is introduced.

4.13 Protected reaction invariants

Definition 4.19 (Protected reaction invariant). Let

$$\mathcal{I}_{\text{prot}} \quad (210)$$

consist of:

1. the persistent atom universe $\mathbb{A}$;
2. the element and isotope maps;
3. the inherited chrysene carbon-skeleton edges outside the declared bond-change set;
4. the chrysene locant identities;
5. the distinguished identities c_α , c_β , o_6 , and $o_{2'}$;
6. adenosine/ribose connectivity outside the declared acyl-transfer support; and
7. every remote substituent edge not contained in the pattern support of the selected reaction grammar.

A reaction path is $\mathcal{I}_{\text{prot}}$ -preserving when all these data remain invariant.

4.14 Reference initial and target graph conditions

For the initial state S_0^Λ , the principal local bonds satisfy

$$\begin{aligned} \bar{b}_{G_0}(v_6, o_6) &= 1, & \bar{b}_{G_0}(o_6, c_\alpha) &= 1, \\ \bar{b}_{G_0}(c_\alpha, c_\beta) &= 1, & \bar{b}_{G_0}(c_\beta, o_\beta) &= 1, \end{aligned} \quad (211)$$

while

$$\bar{b}_{G_0}(v_5, c_\alpha) = 0, \quad \bar{b}_{G_0}(c_\beta, o_{2'}) = 0. \quad (212)$$

For a principal target graph $G_\star^{\text{main}}$, the target conditions include

$$\begin{aligned} \bar{b}_{G_\star}(v_5, c_\alpha) &= 1, \\ \bar{b}_{G_\star}(c_\alpha, n_\alpha) &= 1, \\ \bar{b}_{G_\star}(c_\beta, o_{\text{carbonyl}}) &= 2, \\ \bar{b}_{G_\star}(c_\beta, o_{2'}) &= 1. \end{aligned} \quad (213)$$

The inherited chrysene edge is preserved:

$$\bar{b}_{G_\star}(v_5, v_6) = \bar{b}_{G_0}(v_5, v_6). \quad (214)$$

Thus formation of the new $C5-C_\alpha$ bond does not require cleavage of the inherited $C5-C6$ carbon-framework edge.

4.15 Chemical transition relation

Define

$$S \rightsquigarrow_{\text{chem}} S' \quad (215)$$

when there exists $p \in \mathcal{P}$ and a chemically admissible match such that

$$S \xrightarrow[p]{\text{chem}} S'. \quad (216)$$

Let

$$\rightsquigarrow_{\text{chem}}^* \quad (217)$$

denote its reflexive transitive closure.

Definition 4.20 (Atom-map-preserving reaction path). A finite reaction path

$$S_0 \longrightarrow S_1 \longrightarrow \cdots \longrightarrow S_m \quad (218)$$

is *atom-map preserving* when every state uses the same persistent atom universe and every rewrite preserves the element, isotope, and distinguished atom-identity maps.

Definition 4.21 (Well-formed chemical path). A finite path

$$p : S_0 \longrightarrow S_1 \longrightarrow \cdots \longrightarrow S_m \quad (219)$$

is a *well-formed chemical path* when:

1. every arrow is generated by a rule in $\mathcal{P}$;
2. every rewrite is chemically admissible;
3. every state satisfies $\text{Chem} = 1$;
4. the path is atom-map preserving;
5. $\mathcal{I}_{\text{prot}}$ is preserved;
6. every resource update remains in $\mathcal{R}_{\text{adm}}$; and
7. total charge is conserved.

Let

$$\text{Path}_{\text{chem}}(S, T) \quad (220)$$

denote the set of well-formed finite chemical paths from S to T .

Then

$$S \rightsquigarrow_{\text{chem}}^* T \quad (221)$$

if and only if

$$\text{Path}_{\text{chem}}(S, T) \neq \emptyset. \quad (222)$$

For the realization family introduced in Section 3, the preliminary chemical existence problem is therefore

$$\text{Path}_{\text{chem}}(S_0^\Lambda, S_\star^\Lambda) \neq \emptyset. \quad (223)$$

The stronger problem studied in the remainder of the paper requires each chemical generator to admit a compatible three-dimensional cage lift. Section 5 introduces that geometric refinement.

5 Cage-Constrained Configuration Spaces and Geometric Liftability

Section 4 defines chemically admissible transformations at the level of persistent atom identities and typed molecular graphs. Chemical admissibility alone does not ensure that the atoms participating in a rewrite can occupy a compatible three-dimensional configuration.

The present section therefore introduces a geometric refinement of chemical reachability. Its fundamental distinction is

$$S \rightsquigarrow_{\text{chem}} S' \not\equiv S \rightsquigarrow_C S'. \quad (224)$$

The relation $\rightsquigarrow_C$ will require a chemically admissible graph rewrite together with a continuous geometric lift satisfying the declared cage constraints.

5.1 Embedded configurations and cage support

Let

$$S = (G, \iota, q, r, s, \chi, \rho, \mathcal{K}) \quad (225)$$

be a chemical state with finite atom set

$$V = V(G). \quad (226)$$

Define the unrestricted embedded configuration space

$$\text{Emb}(V) := \{x : V \longrightarrow \mathbb{R}^3 : x \text{ is injective}\}. \quad (227)$$

The proper Euclidean group

$$SE(3) = SO(3) \ltimes \mathbb{R}^3 \quad (228)$$

acts on $\text{Emb}(V)$ by

$$(R, t) \cdot x : v \longmapsto Rx(v) + t. \quad (229)$$

The reduced molecular configuration space is

$$\text{Conf}(V) := \text{Emb}(V)/SE(3). \quad (230)$$

Improper Euclidean transformations are not quotiented out because they may reverse stereochemical orientation.

Let

$$U_{\text{rxn}} \subseteq V \quad (231)$$

denote the completed local chemical reaction support associated with the selected rule family.

Definition 5.1 (Cage support). A *cage support* for S is a finite atom set

$$C(S) \subseteq V \quad (232)$$

such that

$$U_{\text{rxn}} \subseteq C(S) \quad (233)$$

and every atom whose position enters a declared geometric constraint belongs to $C(S)$.

Thus

$$U_{\text{rxn}} \subseteq C(S), \quad (234)$$

usually strictly.

Atoms in $C(S) \setminus U_{\text{rxn}}$ may constrain reaction geometry without undergoing any chemical rewrite.

Restriction of an embedded configuration to the finite cage support induces a projection

$$\pi_C : \text{Conf}(V) \longrightarrow \text{Conf}(C(S)). \quad (235)$$

The finite-dimensional space

$$\text{Conf}(C(S)) \quad (236)$$

will carry the hard geometric constraints used below.

5.2 Geometric observables

For atoms $u, v \in C(S)$, define

$$d_{uv}(x) := \|x(u) - x(v)\|_2. \quad (237)$$

For distinct $u, v, w \in C(S)$, define

$$\theta_{uvw}(x) := \arccos \left(\frac{\langle x(u) - x(v), x(w) - x(v) \rangle}{d_{uv}(x)d_{vw}(x)} \right) \quad (238)$$

whenever the denominator is nonzero.

For $u, v, w, z \in C(S)$, define the oriented volume

$$\Omega_{u,v,w,z}(x) := \det [x(v) - x(u), x(w) - x(u), x(z) - x(u)]. \quad (239)$$

Because proper Euclidean transformations preserve orientation,

$$\text{sgn } \Omega_{u;v,w,z} \quad (240)$$

is well defined on $\text{Conf}(C(S))$.

The stack observables

$$d_\pi, \quad s_\pi, \quad \Theta_\pi \quad (241)$$

retain their definitions from Section 3.3.

5.3 Hard cage constraints and admissible configuration sets

Let

$$J_S \quad (242)$$

be a finite index set.

For each $j \in J_S$, let

$$F_j^S : \text{Conf}(C(S)) \rightarrow \mathbb{R} \quad (243)$$

be a continuous hard-constraint functional.

Equality constraints, when required, are represented by continuous maps

$$H_k^S : \text{Conf}(C(S)) \rightarrow \mathbb{R}. \quad (244)$$

Definition 5.2 (Projected cage-admissible set). The *projected cage-admissible set* of S is

$$\mathcal{K}_C(S) := \bigcap_{j \in J_S} \{x : F_j^S(x) \leq 0\} \cap \bigcap_{k \in K_S} \{x : H_k^S(x) = 0\}. \quad (245)$$

The corresponding full-state admissible set is

$$\mathcal{K}(S) := \{x \in \text{Conf}(V) : \pi_C(x) \in \mathcal{K}_C(S)\}. \quad (246)$$

Definition 5.3 (Cage-realizable state). A chemical state S is *cage realizable* when

$$\mathcal{K}(S) \neq \emptyset. \quad (247)$$

The finite support $C(S)$ is the domain relevant to local cage comparisons. Atoms outside $C(S)$ may be retained in the complete molecular state without entering the local geometric predicates.

5.4 Reference constraint families

The reference realization uses the hard-constraint family

$$\mathfrak{F}_{\text{ref}} = \mathfrak{F}_{\text{ex}} \cup \mathfrak{F}_{\text{tet}} \cup \mathfrak{F}_\pi \cup \mathfrak{F}_{\text{cap}} \cup \mathfrak{F}_\chi \cup \mathfrak{F}_{\text{tr}} \cup \mathfrak{F}_{\text{aux}}. \quad (248)$$

Here:

$\mathfrak{F}_{\text{ex}}$ = excluded-volume constraints,

$\mathfrak{F}_{\text{tet}}$ = tether-span and orientation constraints,

$\mathfrak{F}_\pi$ = π -stack constraints,

$\mathfrak{F}_{\text{cap}} = C5 - C_\alpha$ capture constraints, (249)

$\mathfrak{F}_\chi$ = stereochemical approach constraints,

$\mathfrak{F}_{\text{tr}}$ = terminal acyl-transfer constraints,

$\mathfrak{F}_{\text{aux}}$ = optional auxiliary geometric constraints.

The complete component inequalities are collected in Appendix C. Only the constraints entering the central existence and stereochemical theorems are repeated below.

5.5 π -stack and tether constraints

The reference stack condition is

$$d_\pi(x) \in I_d, \quad s_\pi(x) \in I_s, \quad \Theta_\pi(x) \in I_\theta. \quad (250)$$

For a tether path

$$\mathcal{T} = (a_0, \dots, a_m), \quad (251)$$

define

$$L_{\mathcal{T}}(x) := d_{a_0 a_m}(x), \quad (252)$$

and impose

$$L_{\mathcal{T}}(x) \in I_{\mathcal{T}}. \quad (253)$$

Where the local orientation variable π_ℓ is used, one may additionally require

$$\pi_\ell(x) \in I_\pi. \quad (254)$$

These are geometric constraints only; energetic interpretation belongs to a separately declared realization model.

5.6 Capture geometry

Define the capture distance

$$d_{\text{cap}}(x) := d_{v_5 c_\alpha}(x). \quad (255)$$

Let

$$u_5^{\text{out}}(x) \in \mathbb{S}^2 \quad (256)$$

be a realization-specific reactive direction at v_5 , and define

$$u_{\alpha \rightarrow 5}(x) := \frac{x(v_5) - x(c_\alpha)}{d_{v_5 c_\alpha}(x)}. \quad (257)$$

The corresponding capture angle is

$$\theta_{\text{cap}}(x) := \arccos(\langle u_{\alpha \rightarrow 5}(x), -u_5^{\text{out}}(x) \rangle). \quad (258)$$

Definition 5.4 (Capture-admissible configuration). A configuration is $C5 - C_\alpha$ capture admissible when

$$d_{\text{cap}}(x) \in I_{\text{cap}}^d \quad (259)$$

and

$$\theta_{\text{cap}}(x) \in I_{\text{cap}}^\theta. \quad (260)$$

5.7 Acyl-transfer geometry

For a state containing an activated c_β acyl center, define

$$d_{\text{acyl}}(x) := d_{c_\beta o_{2'}}(x). \quad (261)$$

Let

$$o_{\text{C=O}} \quad (262)$$

denote the carbonyl oxygen in that state and define

$$\theta_{\text{acyl}}(x) := \theta_{o_{\text{C=O}}, c_\beta, o_{2'}}(x). \quad (263)$$

Definition 5.5 (Acyl-transfer-admissible configuration). A configuration is *acyl-transfer admissible* when

$$d_{\text{acyl}}(x) \in I_{\text{acyl}}^d \quad (264)$$

and

$$\theta_{\text{acyl}}(x) \in I_{\text{acyl}}^\theta, \quad (265)$$

together with any explicitly declared proton-transfer or leaving-group orientation conditions.

Because $o_{2'}$ is a persistent atom identity, the transfer geometry is atom-map resolved.

5.8 Stereochemical attack geometry

Consider a state in which

$$\bar{b}(v_5, c_\alpha) = 1 \quad (266)$$

and

$$\bar{b}(c_\alpha, c_\beta) = 1. \quad (267)$$

Define

$$e_1(x) := \frac{x(v_5) - x(c_\alpha)}{d_{v_5 c_\alpha}(x)}. \quad (268)$$

Let

$$\tilde{e}_2(x) := x(c_\beta) - x(c_\alpha), \quad (269)$$

and define

$$e_2(x) := \frac{\tilde{e}_2 - \langle \tilde{e}_2, e_1 \rangle e_1}{\|\tilde{e}_2 - \langle \tilde{e}_2, e_1 \rangle e_1\|} \quad (270)$$

whenever the denominator is nonzero.

Set

$$e_3(x) := e_1(x) \times e_2(x). \quad (271)$$

The oriented local frame is therefore

$$\mathcal{F}_\alpha(x) = (e_1(x), e_2(x), e_3(x)). \quad (272)$$

For an amino-installation approach direction

$$u_{\text{att}} \in \mathbb{S}^2, \quad (273)$$

define

$$\zeta_\chi(x, u_{\text{att}}) := \langle u_{\text{att}}, e_3(x) \rangle \quad (274)$$

and

$$\sigma_\alpha(x, u_{\text{att}}) := \text{sgn } \zeta_\chi(x, u_{\text{att}}). \quad (275)$$

For a robustness parameter $\delta_\chi > 0$, define the two attack regions

$$\mathcal{A}_\alpha^+(\delta_\chi; x) = \{u \in \mathbb{S}^2 : \langle u, e_3(x) \rangle \geq \delta_\chi\}, \quad (276)$$

and

$$\mathcal{A}_\alpha^-(\delta_\chi; x) = \{u \in \mathbb{S}^2 : \langle u, e_3(x) \rangle \leq -\delta_\chi\}. \quad (277)$$

The margin δ_χ excludes trajectories arbitrarily close to the separating plane.

Let

$$\kappa_\alpha : \{-1, +1\} \longrightarrow \{R, S\} \quad (278)$$

be the realization-specific map assigning the geometric attack side to the final absolute configuration after the complete product substituent ordering has been specified.

For target configuration $\chi_\star$, let

$$\sigma_\star \in \{-1, +1\} \quad (279)$$

satisfy

$$\kappa_\alpha(\sigma_\star) = \chi_\star, \quad (280)$$

and define

$$\mathcal{A}_{\chi_\star}(\delta_\chi; x) := \mathcal{A}_\alpha^{\sigma_\star}(\delta_\chi; x). \quad (281)$$

5.9 Strong and energetic stereochemical selection

Let

$$\mathcal{U}_N(x) \subseteq \mathbb{S}^2 \quad (282)$$

be the set of nitrogen-approach directions admitted by the cage at x .

Definition 5.6 (Strong cage stereoselectivity). The cage is *strongly $\chi_\star$ -selective* at x when

$$\mathcal{U}_N(x) \cap \mathcal{A}_{\chi_\star}(\delta_\chi; x) \neq \emptyset \quad (283)$$

and

$$\mathcal{U}_N(x) \cap \mathcal{A}_{\chi_{\text{opp}}}(\delta_\chi; x) = \emptyset. \quad (284)$$

Proposition 5.7 (Deterministic stereochemical consequence). *Suppose the amino-installation rewrite is stereospecific with respect to the local attack sign σ_α , and suppose the cage is strongly $\chi_\star$ -selective throughout the relevant transition region.*

Then every cage-admissible realization of that rewrite produces

$$\chi(c_\alpha) = \chi_\star. \quad (285)$$

Proof. Every admissible approach direction lies in the attack branch mapped by κ_α to $\chi_\star$, while the opposite branch is excluded. Stereospecificity of the rewrite therefore fixes the product configuration. $\square$

For a physical realization in which both branches remain geometrically accessible, one may instead define

$$\Delta\Delta G_\chi^\ddagger := \Delta G_{\text{opp}}^\ddagger - \Delta G_\star^\ddagger. \quad (286)$$

The condition

$$\Delta\Delta G_\chi^\ddagger > 0 \quad (287)$$

represents an energetic preference rather than deterministic geometric exclusion.

5.10 Soft constraints and compact cage-support domains

In addition to hard admissibility constraints, a realization may assign a continuous soft cage functional

$$\mathcal{E}_{\text{cage}}^S : \mathcal{K}_C(S) \longrightarrow \mathbb{R}. \quad (288)$$

For example,

$$\mathcal{E}_{\text{cage}} = E_\pi + E_{\text{tether}} + E_{\text{HB}} + E_{\text{el}} + E_{\text{strain}}, \quad (289)$$

with realization-specific definitions of the component terms.

The symbol $\mathcal{E}_{\text{cage}}$ does not require the functional to equal an exact molecular free energy.

The compactness statement applies to the finite cage-support configuration space, not automatically to the complete molecular configuration space.

Lemma 5.8 (Compactness of the projected cage domain). *Fix a proper-Euclidean gauge on $C(S)$ by holding three non-collinear reference atoms at fixed coordinates. Assume:*

1. *every atom of $C(S)$ is confined to a closed bounded subset of $\mathbb{R}^3$;*
2. *positive lower-distance constraints prevent collisions of distinct atoms in the gauge-fixed cage support;*
3. *all hard constraint functionals are continuous; and*
4. *$\mathcal{K}_C(S)$ is defined by finitely many closed equalities*

and inequalities.

Then the gauge-fixed projected cage domain

$$\tilde{\mathcal{K}}_C(S) \quad (290)$$

is compact.

Proof. After gauge fixing, coordinates of the finite atom set $C(S)$ lie in a finite-dimensional Euclidean space. The bounded-coordinate hypothesis gives boundedness. The hard inequalities, equalities, and positive noncollision conditions define a closed subset of that bounded domain. The result therefore follows from the Heine–Borel theorem. $\square$

Corollary 5.9 (Existence of a minimum soft cage functional). *Under the hypotheses of Lemma 5.8, if*

$$\tilde{\mathcal{K}}_C(S) \neq \emptyset \quad (291)$$

and $\mathcal{E}_{\text{cage}}^S$ is continuous, then there exists

$$x_{\min} \in \tilde{\mathcal{K}}_C(S) \quad (292)$$

such that

$$\mathcal{E}_{\text{cage}}^S(x_{\min}) = \min_{x \in \tilde{\mathcal{K}}_C(S)} \mathcal{E}_{\text{cage}}^S(x). \quad (293)$$

Proof. Apply the extreme-value theorem to the compact set $\tilde{\mathcal{K}}_C(S)$. $\square$

5.11 Transition configuration spaces and geometric lifts

Let

$$p : S \xrightarrow{\text{chem}} S' \quad (294)$$

be a chemically admissible rewrite.

Associate with p a transition configuration space

$$\mathcal{X}_p \quad (295)$$

containing the geometric degrees of freedom required to compare the reactant and product configurations.

Let

$$\mathcal{C}_p \subseteq \mathcal{X}_p \quad (296)$$

be the subset satisfying:

1. all hard cage constraints required to persist during the transformation;
2. rule-specific approach constraints;
3. protected excluded-volume conditions; and
4. any transition-specific stereochemical conditions.

The space $\mathcal{C}_p$ is an admissibility domain. It is not identified with an exact electronic transition-state surface.

Definition 5.10 (Geometric lift). A *geometric lift* of the chemical rewrite p is a continuous map

$$\gamma : [0, 1] \longrightarrow \mathcal{C}_p \quad (297)$$

whose endpoints are compatible with the reactant and product states:

$$\gamma(0) \in \mathcal{K}(S), \quad \gamma(1) \in \mathcal{K}(S'). \quad (298)$$

Define

$$\text{Lift}_{\mathcal{C}}(p; S, S') \quad (299)$$

to be the set of all geometric lifts of p .

Definition 5.11 (Cage-liftable rewrite). A chemically admissible rewrite

$$p : S \xrightarrow{\text{chem}} S' \quad (300)$$

is *cage liftable* when

$$\text{Lift}_{\mathcal{C}}(p; S, S') \neq \emptyset. \quad (301)$$

5.12 Cage-constrained transitions and paths

Definition 5.12 (Cage-constrained transition). For cage-realizable states S, S' , write

$$S \rightsquigarrow_{\mathcal{C}} S' \quad (302)$$

when there exists $p \in \mathcal{P}$ such that:

$$S \xrightarrow[p]{\text{chem}} S', \quad (303)$$

$$\text{Lift}_{\mathcal{C}}(p; S, S') \neq \emptyset.$$

Let

$$\rightsquigarrow_{\mathcal{C}}^* \quad (304)$$

denote the reflexive transitive closure.

Proposition 5.13 (Cage reachability refines chemical reachability). For all states S, T ,

$$S \rightsquigarrow_{\mathcal{C}}^* T \implies S \rightsquigarrow_{\text{chem}}^* T. \quad (305)$$

Proof. Every generating cage-constrained transition is, by definition, a chemically admissible transition. The implication is preserved under finite composition. $\square$

Definition 5.14 (Cage-constrained reaction path). A finite sequence

$$p_{\mathcal{C}} : S_0 \rightsquigarrow_{\mathcal{C}} S_1 \rightsquigarrow_{\mathcal{C}} \cdots \rightsquigarrow_{\mathcal{C}} S_m \quad (306)$$

is a *cage-constrained reaction path*.

Let

$$\text{Path}_{\mathcal{C}}(S, T) \quad (307)$$

denote the set of all finite cage-constrained paths from S to T .

Then

$$S \rightsquigarrow_{\mathcal{C}}^* T \quad (308)$$

if and only if

$$\text{Path}_{\mathcal{C}}(S, T) \neq \emptyset. \quad (309)$$

5.13 Robust cage liftability

Let

$$\gamma \in \text{Lift}_{\mathcal{C}}(p; S, S') \quad (310)$$

and let

$$F_1, \dots, F_N \quad (311)$$

be the finite family of designated hard transition constraints.

Definition 5.15 (Constraint margin). For each constraint F_j , define

$$m_j(\gamma) := - \max_{t \in [0, 1]} F_j(\gamma(t)). \quad (312)$$

Thus

$$m_j(\gamma) > 0 \quad (313)$$

means that the entire lift remains strictly inside the corresponding hard boundary.

Definition 5.16 (Robustly cage-liftable rewrite). A rewrite is *robustly cage liftable* when it possesses a lift γ for which

$$m_j(\gamma) > 0 \quad (314)$$

for every designated robustness constraint.

Lemma 5.17 (Persistence under strict margin). Suppose

$$m_j(\gamma) \geq m_j > 0 \quad (315)$$

for a finite family of continuous constraints. Then there exists a neighborhood of $\gamma([0, 1])$ such that every sufficiently close continuous candidate path remains inside all of the same hard constraint sets.

Proof. The image $\gamma([0, 1])$ is compact. Uniform continuity of the finite constraint family therefore gives a positive perturbation radius smaller than every declared margin. $\square$

The quantitative transported-path form of this principle is developed in Section 7.

5.14 The constrained reachability problem

Combining the chemical and geometric layers, the principal reachability question is now

$$\boxed{\text{Path}_{\mathcal{C}}(S_0^{\Lambda}, S_{\star}^{\Lambda}) \neq \emptyset.} \quad (316)$$

This statement requires:

$$\begin{array}{c} \text{chemical graph admissibility} \\ \Downarrow \\ \text{geometric cage liftability} \\ \Downarrow \\ \text{finite composability.} \end{array} \quad (317)$$

When a stereochemically specified target is required, one additionally imposes

$$\chi(c_{\alpha}) = \chi_{\star}. \quad (318)$$

The next section packages these state and transition data into the cage-constrained reaction category used by the existence and local-invariance theorems.

6 The Cage-Constrained Reaction Category

Sections 4 and 5 provide two complementary structures: chemically admissible local graph transformations and geometric conditions under which those transformations possess cage-compatible lifts.

We now assemble these data into compositional path categories.

The basic hierarchy is

$$\begin{array}{c} \text{chemical states and rewrites} \\ \Downarrow \\ \mathbf{Chem} \\ \text{cage-liftable states and rewrites} \\ \Downarrow \\ \mathbf{Reach}_{\mathcal{C}}. \end{array} \quad (319)$$

The categories are directed path categories. No inverse transformation is assumed merely because a forward transformation exists.

The free-category construction also retains the ordered reaction word: different rules, matches, or rule orderings remain distinct morphisms unless an explicit quotient is introduced.

6.1 State universes and transition quivers

Fix a closed reaction universe

$$\Omega_{\text{rxn}} \quad (320)$$

with persistent atom universe $\mathbb{A}$, element map ϵ , resource ledger, and protected invariant $\mathcal{I}_{\text{prot}}$ as defined in Section 4.

Let

$$\mathbf{St}_{\text{chem}} \quad (321)$$

denote the class of chemical states

$$S = (G, \iota, q, r, s, \chi, \rho, \mathcal{K}) \quad (322)$$

over Ω_{rxn} satisfying

$$\text{Chem}(S) = 1 \quad (323)$$

and the declared protected-state conditions.

Define the cage-realizable state class

$$\mathbf{St}_{\mathcal{C}} := \{S \in \mathbf{St}_{\text{chem}} : \mathcal{K}(S) \neq \emptyset\}. \quad (324)$$

Thus

$$\mathbf{St}_{\mathcal{C}} \subseteq \mathbf{St}_{\text{chem}}. \quad (325)$$

Let

$$\mathcal{P} = \{p_{\gamma}\}_{\gamma \in \Gamma} \quad (326)$$

be the reaction grammar of Section 4.12.

Definition 6.1 (Elementary chemical transition). An *elementary chemical transition* is a tuple

$$e = (S, p, m, S') \quad (327)$$

such that

$$S \xrightarrow[p, m]{\text{chem}} S'. \quad (328)$$

Its source and target are

$$s(e) = S, \quad t(e) = S'. \quad (329)$$

The explicit match m is part of the transition data. Applications of one abstract rule at different labeled sites are therefore distinct elementary transitions.

Let

$$\mathbf{E}_{\text{chem}} \quad (330)$$

denote the class of elementary chemical transitions. The chemical transition quiver is

$$\mathbf{Q}_{\text{chem}} = (\mathbf{St}_{\text{chem}}, \mathbf{E}_{\text{chem}}, s, t). \quad (331)$$

Definition 6.2 (Elementary cage-constrained transition). An elementary chemical transition

$$e = (S, p, m, S') \quad (332)$$

is an *elementary cage-constrained transition* when

$$S, S' \in \text{St}_{\mathcal{C}} \quad (333)$$

and

$$\text{Lift}_{\mathcal{C}}(p; S, S') \neq \emptyset. \quad (334)$$

Let

$$\mathbf{E}_{\mathcal{C}} \subseteq \mathbf{E}_{\text{chem}} \quad (335)$$

be the resulting class of elementary cage transitions.

The cage transition quiver is

$$\mathbf{Q}_{\mathcal{C}} = (\text{St}_{\mathcal{C}}, \mathbf{E}_{\mathcal{C}}, s, t). \quad (336)$$

6.2 Chemical and cage-constrained path categories

Definition 6.3 (Chemical path category). The *chemical path category* is the free category

$$\mathbf{Chem} := \text{Free}(\mathbf{Q}_{\text{chem}}). \quad (337)$$

Its objects are

$$\text{Ob}(\mathbf{Chem}) = \text{St}_{\text{chem}}. \quad (338)$$

A nonidentity morphism

$$f : S \longrightarrow T \quad (339)$$

is a finite composable word

$$f = e_n \cdots e_2 e_1 \quad (340)$$

with

$$s(e_1) = S, \quad t(e_n) = T, \quad (341)$$

and

$$t(e_i) = s(e_{i+1}) \quad (1 \leq i < n). \quad (342)$$

The empty word

$$1_S : S \longrightarrow S \quad (343)$$

is the identity, and composition is path concatenation.

Hence

$$\text{Hom}_{\mathbf{Chem}}(S, T) \cong \text{Path}_{\text{chem}}(S, T). \quad (344)$$

Definition 6.4 (Cage-constrained reaction category). The *cage-constrained reaction category* is

$$\mathbf{Reach}_{\mathcal{C}} := \text{Free}(\mathbf{Q}_{\mathcal{C}}). \quad (345)$$

Thus

$$\text{Ob}(\mathbf{Reach}_{\mathcal{C}}) = \text{St}_{\mathcal{C}}. \quad (346)$$

For $S, T \in \text{St}_{\mathcal{C}}$,

$$\text{Hom}_{\mathbf{Reach}_{\mathcal{C}}}(S, T) \cong \text{Path}_{\mathcal{C}}(S, T). \quad (347)$$

Corollary 6.5 (Categorical cage reachability). For $S, T \in \text{St}_{\mathcal{C}}$,

$$S \rightsquigarrow_{\mathcal{C}}^* T \quad (348)$$

if and only if

$$\text{Hom}_{\mathbf{Reach}_{\mathcal{C}}}(S, T) \neq \emptyset. \quad (349)$$

Equation (349) is the categorical form of the existence statement used in the main theorems.

6.3 Chemical support, pattern footprint, and local categories

The revised local theory distinguishes atoms that actually change from atoms that are merely required for rule matching.

For an elementary transition

$$e = (S, p, m, S'), \quad (350)$$

define its change support by

$$\text{Supp}(e) := \text{supp}(S, S'). \quad (351)$$

Using the persistent vertex correspondence of the rule, define its *pattern footprint*

$$\text{Foot}(e) := m(\text{Pat}(p)). \quad (352)$$

Thus

$$\text{Supp}(e) \subseteq \text{Foot}(e). \quad (353)$$

For a finite path

$$f = e_n \cdots e_1, \quad (354)$$

define

$$\text{Supp}(f) := \bigcup_{i=1}^n \text{Supp}(e_i) \quad (355)$$

and

$$\text{Foot}(f) := \bigcup_{i=1}^n \text{Foot}(e_i). \quad (356)$$

For identity morphisms,

$$\text{Supp}(1_S) = \text{Foot}(1_S) = \emptyset. \quad (357)$$

Lemma 6.6 (Local footprints under composition).
For composable morphisms

$$f : S \longrightarrow T, \quad g : T \longrightarrow U, \quad (358)$$

one has

$$\text{Supp}(g \circ f) = \text{Supp}(f) \cup \text{Supp}(g) \quad (359)$$

and

$$\text{Foot}(g \circ f) = \text{Foot}(f) \cup \text{Foot}(g). \quad (360)$$

Proof. Composition in the free category is concatenation of elementary transition words. Both sets are therefore the unions over the constituent generators. $\square$

Let

$$U \subseteq \mathbb{A} \quad (361)$$

be a declared local reaction domain.

Definition 6.7 (Local chemical path category). The category

$$\mathbf{Chem}[U] \quad (362)$$

is the wide subcategory of $\mathbf{Chem}$ generated by elementary chemical transitions satisfying

$$\text{Foot}(e) \subseteq U. \quad (363)$$

Definition 6.8 (Local cage-constrained reaction category). The category

$$\mathbf{Reach}_C[U] \quad (364)$$

is the wide subcategory of $\mathbf{Reach}_C$ generated by elementary cage transitions satisfying

$$\text{Foot}(e) \subseteq U. \quad (365)$$

A morphism belongs to either local category exactly when its pattern footprint is contained in U .

For the canonical rule family,

$$\text{Foot}(\Phi_{\text{can}}) \subseteq U_{\text{rxn}}, \quad (366)$$

so the canonical witness, when cage liftable, belongs to

$$\mathbf{Reach}_C[U_{\text{rxn}}]. \quad (367)$$

Using pattern footprint rather than only changed-atom support ensures that every atom whose chemical state is inspected by a local rule is included in the declared locality domain.

6.4 Chemical forgetful functor and reachability preorder

Every elementary cage transition is an elementary chemical transition. The inclusion of transition quivers therefore induces a canonical functor

$$\mathcal{U}_{\text{chem}} : \mathbf{Reach}_C \longrightarrow \mathbf{Chem}. \quad (368)$$

On objects,

$$\mathcal{U}_{\text{chem}}(S) = S, \quad (369)$$

and on elementary transitions,

$$\mathcal{U}_{\text{chem}}(S, p, m, S') = (S, p, m, S'). \quad (370)$$

Thus the functor forgets the requirement of geometric liftability but retains the chemical transition word.

Proposition 6.9 (Faithfulness of the chemical forgetful functor). *The functor*

$$\mathcal{U}_{\text{chem}} : \mathbf{Reach}_C \longrightarrow \mathbf{Chem} \quad (371)$$

is faithful and need not be full.

Proof. Morphisms in both free categories are finite words in their generating transitions. The inclusion preserves every cage-transition word and therefore does not identify distinct source morphisms.

It is not generally full because $\mathbf{Chem}$ may contain chemically admissible transitions or paths having no cage-liftable counterpart. $\square$

For endpoint existence, define

$$S \preceq_C T \quad (372)$$

if and only if

$$\text{Hom}_{\mathbf{Reach}_C}(S, T) \neq \emptyset. \quad (373)$$

Proposition 6.10 (Cage reachability is a preorder). *The relation $\preceq_C$ is reflexive and transitive.*

Proof. Reflexivity follows from $1_S : S \rightarrow S$. If

$$S \preceq_C T \quad \text{and} \quad T \preceq_C U,$$

choose morphisms

$$f : S \rightarrow T, \quad g : T \rightarrow U.$$

Then

$$g \circ f : S \rightarrow U,$$

so $S \preceq_C U$. $\square$

Antisymmetry is not imposed; distinct chemical states may be mutually reachable.

6.5 Reaction-word nonuniqueness

Because $\mathbf{Reach}_C$ is free on the elementary cage-transition quiver, two morphisms

$$f = e_n \cdots e_1, \quad g = e'_m \cdots e'_1 \quad (374)$$

are equal precisely when their ordered elementary-transition words are equal.

Distinct reaction rules, labeled matches, or rule orderings therefore define distinct morphisms.

Definition 6.11 (Reaction-word distinctness). Two morphisms

$$f, g : S \longrightarrow T \quad (375)$$

are *reaction-word distinct* when

$$f \neq g \quad (376)$$

as morphisms of $\mathbf{Reach}_C$.

Definition 6.12 (Reaction-word nonuniqueness). A target T is *reaction-word nonunique relative to S* when

$$\boxed{\# \text{Hom}_{\mathbf{Reach}_C}(S, T) \geq 2.} \quad (377)$$

This is a statement about the declared reaction grammar. The geometric lift itself is not part of the morphism data, so Equation (377) does not count distinct continuous geometric trajectories associated with one generator word and does not rank the physical probability of the resulting reaction pathways.

A physical interpretation of distinct reaction words requires the additional realization and certification information developed later.

6.6 Target-family reachability

Let

$$\mathfrak{T} \subseteq \text{St}_C \quad (378)$$

be any declared family of terminal states.

Definition 6.13 (Target-family reachability). The target family $\mathfrak{T}$ is *reachable from S* when

$$\exists T \in \mathfrak{T} \text{ such that } S \preceq_C T. \quad (379)$$

Equivalently,

$$\exists T \in \mathfrak{T} \text{ such that } \text{Hom}_{\mathbf{Reach}_C}(S, T) \neq \emptyset. \quad (380)$$

This formulation allows a reachability theorem to specify the principal product while leaving nonessential terminal coproduct choices within an admissible target class.

The connectivity and stereochemical target families used by the main existence theorem are defined in Section 9.

6.7 Realization-indexed reaction categories

The chemical grammar, cage constraints, and resulting transition quiver may depend on realization data.

Let

$$\mathbf{p} \quad (381)$$

denote a realization parameter tuple containing, as applicable, substitution context, adenine anchor, source-capture ordering, cage windows, charge/electronic state, and resource data.

Write

$$\mathbf{Chem}^{\mathbf{p}} \quad (382)$$

and

$$\mathbf{Reach}_C^{\mathbf{p}} \quad (383)$$

for the corresponding chemical and cage-constrained path categories.

For the reference $C6 \rightarrow C5$, $C2$ -anchored realization with substitution context Λ , write

$$\boxed{\mathbf{Reach}_{\Lambda}^{6 \rightarrow 5}} \quad (384)$$

for the associated cage-constrained reaction category, and similarly

$$\mathbf{Chem}_{\Lambda}^{6 \rightarrow 5} \quad (385)$$

for its chemical path category.

When local support must be displayed explicitly, write

$$\mathbf{Reach}_{\Lambda}^{6 \rightarrow 5}[U_{\text{rxn}}] \quad (386)$$

and

$$\mathbf{Chem}_{\Lambda}^{6 \rightarrow 5}[U_{\text{rxn}}]. \quad (387)$$

For the paired $C5 \rightarrow C6$ realization introduced later, the corresponding notation is

$$\mathbf{Reach}_{\Lambda}^{5 \rightarrow 6}. \quad (388)$$

No equivalence between $\mathbf{Reach}_{\Lambda}^{6 \rightarrow 5}$ and $\mathbf{Reach}_{\Lambda}^{5 \rightarrow 6}$ is assumed by notation alone.

6.8 Local generator transport

Let

$$U, \tilde{U} \subseteq \mathbb{A} \quad (389)$$

be labeled local reaction domains, and suppose

$$\varphi : U \longrightarrow \tilde{U} \quad (390)$$

is a bijection preserving the local data required by the selected grammar, including:

1. element type;
2. distinguished atom role;
3. relevant bond labels;
4. formal-charge and local electronic classes;
5. stereochemical reference data; and
6. rule-pattern incidence data.

For a local rule p with

$$\text{Pat}(p) \subseteq U, \quad (391)$$

define the transported rule

$$\varphi_* p \quad (392)$$

by relabeling the complete local rule datum through φ .

For an elementary transition

$$e = (S, p, m, S'), \quad (393)$$

write

$$\varphi_* e = (\tilde{S}, \varphi_* p, \varphi_* m, \tilde{S}') \quad (394)$$

whenever the corresponding source and target states are defined.

Definition 6.14 (Cage-compatible generator transport). A local identification φ is *cage compatible* for an elementary cage transition e when the transported transition

$$\varphi_* e \quad (395)$$

is also an elementary cage transition in the target realization.

Proposition 6.15 (Extension of generator transport). Suppose a local state identification and support bijection φ :

1. transport every generator of $\widetilde{\text{Reach}}_C[U]$ to a cage-compatible generator of $\widetilde{\text{Reach}}_C[\tilde{U}]$; and
2. preserve source and target under the corresponding state identification.

Then the generator assignment extends uniquely to a functor

$$\Phi_\varphi : \text{Reach}_C[U] \longrightarrow \widetilde{\text{Reach}}_C[\tilde{U}]. \quad (396)$$

Proof. The source category is free on its local transition quiver. A source–target-compatible map on objects and generating edges therefore extends uniquely to a functor on finite edge words. $\square$

For

$$f = e_n \cdots e_1, \quad (397)$$

the transported path is

$$\Phi_\varphi(f) = \Phi_\varphi(e_n) \cdots \Phi_\varphi(e_1). \quad (398)$$

Corollary 6.16 (Local transport preserves reachability). Under the hypotheses of Proposition 6.15,

$$S \preceq_C T \quad (399)$$

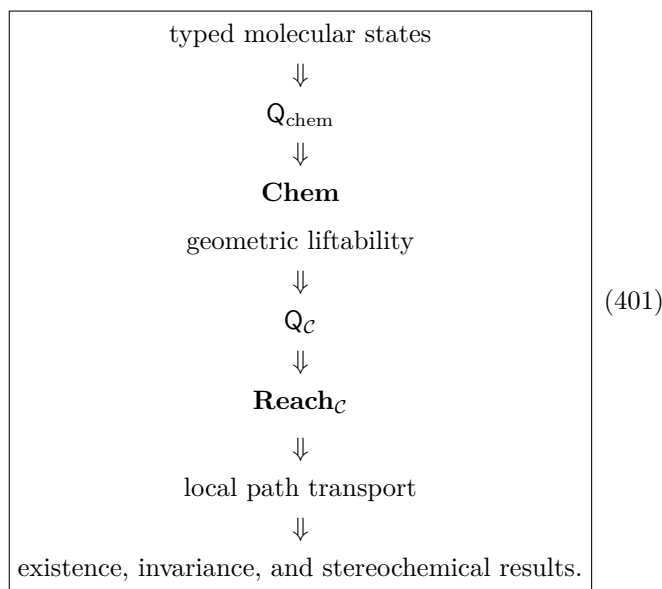
through the local source category implies

$$\Phi_\varphi(S) \preceq_{\tilde{C}} \Phi_\varphi(T). \quad (400)$$

The exact and perturbative context-extension results of Section 7 supply concrete sufficient conditions for constructing such transported paths across the chrysene substitution family. The same universal property will later be used for the dual-cipher and anchor-transport constructions.

6.9 Categorical form of the theorem program

The structures required by the remainder of the paper may now be summarized as



The next section determines when a path in a local reaction category can be transported across changes in remote molecular context.

7 Locality, Context Extension, and Substitution Invariance

The reaction category of Section 6 retains the complete molecular state, whereas the transformations of primary interest are supported on a finite neighborhood of the C5/C6 reactive pair. The purpose of the present section is to determine which parts of a reaction path remain invariant

when the molecular context outside that neighborhood is changed.

Two questions must be separated:

Does the same local chemical rewrite remain defined?

$\Downarrow$

Does a corresponding three-dimensional path remain cage admissible?

(402)

The first question is combinatorial and admits an exact context-extension theorem. The second is geometric. It requires a corresponding candidate geometric transport together with sufficient margin from the cage-constraint boundary.

Accordingly,

$$\boxed{\text{local chemical invariance} \not\Rightarrow \text{local cage invariance.}} \quad (403)$$

The principal application is the substitution family

$$\mathcal{L} = \{\{6, 12\}, \{3, 6, 12\}, \{3, 6, 9, 12\}\}. \quad (404)$$

7.1 Completed local reaction support

Let

$$U_6 \subseteq \mathbb{A} \quad (405)$$

denote the C5/C6-centered structural reaction support introduced previously.

For a local rule $p \in \mathcal{P}$, let

$$\text{Act}(p) \quad (406)$$

denote the set of persistent atom identities whose bond incidences, bond labels, formal charges, radical labels, or stereochemical labels may change under p .

Fix a selected local reaction grammar

$$\mathcal{P}_6 \subseteq \mathcal{P}. \quad (407)$$

Definition 7.1 (Completed reaction support). The *completed local reaction support* of $\mathcal{P}_6$ is

$$U_{\text{rxn}} := U_6 \cup \bigcup_{p \in \mathcal{P}_6} \text{Act}(p). \quad (408)$$

Thus every atom whose chemical state may be altered by the selected grammar belongs to U_{rxn} . For the canonical witness of Section 8, this includes any explicitly mapped oxygen donor, nitrogen donor, hydrogen, proton-transfer atom, or other reagent atom that participates directly in a rewrite.

For a realization with substitution pattern $\Lambda \in \mathcal{L}$, write

$$\mathbb{A}^\Lambda = U_{\text{rxn}} \sqcup X^\Lambda, \quad (409)$$

where X^Λ is the *external context*.

The external context may contain remote chrysene substituents, additional cage atoms, stacking partners, counterions, or other realization-specific structures.

7.2 Exact local chemical equivalence

Definition 7.2 (Local chemical restriction). For a state S^Λ , the restriction

$$\text{Res}_{U_{\text{rxn}}}(S^\Lambda) \quad (410)$$

is the complete chemical-state datum induced on U_{rxn} , including:

1. the labeled molecular graph;
2. formal-charge and radical labels;
3. local electronic-state labels required by $\mathcal{P}_6$;
4. stereochemical labels; and
5. resource labels explicitly referenced by the local grammar.

The full cage geometry is not included in $\text{Res}_{U_{\text{rxn}}}$.

Definition 7.3 (Exact local chemical equivalence). Two states

$$S^\Lambda, \quad S^{\Lambda'} \quad (411)$$

are *exactly chemically equivalent on U_{rxn}* when there exists a persistent-label-preserving isomorphism

$$\varphi_U : U_{\text{rxn}}^\Lambda \longrightarrow U_{\text{rxn}}^{\Lambda'} \quad (412)$$

such that

$$\varphi_U(\text{Res}_{U_{\text{rxn}}} S^\Lambda) = \text{Res}_{U_{\text{rxn}}} S^{\Lambda'}. \quad (413)$$

For the remote-substitution comparison considered here, persistent local atom labels are canonically identified. We therefore abbreviate

$$S^\Lambda \equiv_{U_{\text{rxn}}} S^{\Lambda'}. \quad (414)$$

Definition 7.4 (Reaction-inert external context). The external context X^Λ is *reaction inert relative to $\mathcal{P}_6$* when, for every $p \in \mathcal{P}_6$:

1. $\text{Act}(p) \subseteq U_{\text{rxn}}$;
2. no bond incident to an atom of X^Λ is changed;
3. no formal-charge, radical, electronic, or stereochemical label on X^Λ is changed; and
4. no chemical matching condition of p refers to chemical state data in X^Λ .

Reaction inertness is a chemical condition only. Atoms in X^Λ may still influence cage geometry and therefore affect geometric liftability.

7.3 Exact chemical context extension

Lemma 7.5 (Single-step context extension). *Suppose*

$$S^\Lambda \equiv_{U_{\text{rxn}}} S^{\Lambda'} \quad (415)$$

and

$$e = (S^\Lambda, p, m, T^\Lambda) \quad (416)$$

is a chemically admissible elementary transition satisfying

$$\text{Supp}(e) \subseteq U_{\text{rxn}}. \quad (417)$$

If the external context of $S^{\Lambda'}$ is reaction inert relative to p , then there exists a corresponding chemically admissible transition

$$e' = (S^{\Lambda'}, p', m', T^{\Lambda'}) \quad (418)$$

such that

$$T^\Lambda \equiv_{U_{\text{rxn}}} T^{\Lambda'}, \quad (419)$$

while the external context remains unchanged.

Proof. Transport the reactant pattern, preserved interface, product pattern, and match through φ_U . Exact local chemical equivalence supplies the corresponding reactant pattern in $S^{\Lambda'}$.

Because $\text{Supp}(e) \subseteq U_{\text{rxn}}$, the rule changes no chemical datum in the external context. The transported local rewrite therefore glues uniquely to the unchanged external graph and produces $T^{\Lambda'}$. The induced product-state data on U_{rxn} agree under φ_U . $\square$

Theorem 7.6 (Finite chemical context-extension theorem). *Let*

$$\mathbf{p}^\Lambda : S_0^\Lambda \longrightarrow S_1^\Lambda \longrightarrow \cdots \longrightarrow S_n^\Lambda \quad (420)$$

be a well-formed chemical path with

$$\text{Supp}(\mathbf{p}^\Lambda) \subseteq U_{\text{rxn}}. \quad (421)$$

Suppose

$$S_0^\Lambda \equiv_{U_{\text{rxn}}} S_0^{\Lambda'} \quad (422)$$

and the external context of the Λ' -realization is reaction inert relative to every rule appearing in $\mathbf{p}^\Lambda$.

Then there exists a corresponding path

$$\mathbf{p}^{\Lambda'} : S_0^{\Lambda'} \longrightarrow S_1^{\Lambda'} \longrightarrow \cdots \longrightarrow S_n^{\Lambda'} \quad (423)$$

such that

$$S_i^\Lambda \equiv_{U_{\text{rxn}}} S_i^{\Lambda'} \quad (0 \leq i \leq n). \quad (424)$$

Proof. Apply Lemma 7.5 successively to the finite ordered rewrite word. The external context remains unchanged after every step, so the hypotheses are preserved inductively. $\square$

Corollary 7.7 (Chemical context-extension functor). *Under the hypotheses of Theorem 7.6, transport of local generators extends uniquely to a functor*

$$\mathfrak{E}_{\Lambda \rightarrow \Lambda'} : \mathbf{Chem}^\Lambda[U_{\text{rxn}}] \longrightarrow \mathbf{Chem}^{\Lambda'}[U_{\text{rxn}}]. \quad (425)$$

Hypothesis 7.8 (Local chemical concordance). For every

$$\Lambda, \Lambda' \in \mathcal{L}, \quad (426)$$

the reference initial states satisfy

$$S_0^\Lambda \equiv_{U_{\text{rxn}}} S_0^{\Lambda'}, \quad (427)$$

and all differences among the substitution contexts are reaction inert relative to the selected local grammar $\mathcal{P}_6$.

Theorem 7.9 (Chemical substitution invariance). *Assume Hypothesis 7.8.*

If T^Λ is reachable from S_0^Λ through a chemical path supported in U_{rxn} , then for every $\Lambda' \in \mathcal{L}$ there exists a corresponding state $T^{\Lambda'}$ such that

$$S_0^{\Lambda'} \rightsquigarrow_{\text{chem}}^* T^{\Lambda'} \quad (428)$$

and

$$T^\Lambda \equiv_{U_{\text{rxn}}} T^{\Lambda'}. \quad (429)$$

Proof. Apply Theorem 7.6 to the selected local path. $\square$

Chemical substitution invariance is therefore exact at the graph-rewrite level.

7.4 Exact cage transport

Let

$$C \supseteq U_{\text{rxn}} \quad (430)$$

be the finite cage support relevant to a selected path.

Definition 7.10 (Exact cage concordance). Two corresponding states are *exactly cage concordant* on C when there exists a label-preserving identification of their cage supports under which:

1. their chemical restrictions agree on U_{rxn} ;
2. their declared cage observables correspond up to a proper Euclidean transformation; and
3. the relevant state and transition constraint fami-

lies correspond under that identification.

Theorem 7.11 (Exact cage-context extension). *Let*

$$\mathbf{p}_C^\Lambda : S_0^\Lambda \rightsquigarrow_C \cdots \rightsquigarrow_C S_n^\Lambda \quad (431)$$

be a cage-constrained path supported chemically in U_{rxn} . Suppose:

1. *its chemical path transports by Theorem 7.6;*
2. *corresponding states are exactly cage concordant on C ; and*
3. *all rule-specific transition constraints are preserved by the cage identification.*

Then the transported chemical path is cage constrained:

$$S_0^{\Lambda'} \rightsquigarrow_C \cdots \rightsquigarrow_C S_n^{\Lambda'}. \quad (432)$$

Proof. Each reference geometric lift transports through the exact cage identification. Preservation of the state and transition constraints places the transported path in the corresponding transition-admissible domain. Hence every transported chemical generator remains cage liftable, and finite composition gives the result. $\square$

Exact cage concordance is stronger than required for the substitution applications below.

7.5 Candidate geometric transport and robustness margin

Fix a reference substitution context

$$\Lambda_0 \in \mathcal{L} \quad (433)$$

and a finite cage-constrained path

$$\mathbf{p}_C^{\Lambda_0} = (e_1, \dots, e_n). \quad (434)$$

For each elementary transition choose one geometric lift

$$\gamma_i : [0, 1] \longrightarrow \mathcal{C}_{p_i}^{\Lambda_0}. \quad (435)$$

Let

$$F_{ij}^{\Lambda_0} \leq 0, \quad 1 \leq j \leq N_i, \quad (436)$$

be the finite family of designated hard transition constraints on the i -th lift.

Define

$$m_{ij} := - \max_{t \in [0, 1]} F_{ij}^{\Lambda_0}(\gamma_i(t)). \quad (437)$$

Definition 7.12 (Uniform positive cage margin). The selected reference path has a *uniform positive cage*

margin when

$$m_{\min} := \min_{i,j} m_{ij} > 0. \quad (438)$$

Let $\Lambda \in \mathcal{L}$ be another realization whose chemical path has been transported by Theorem 7.6.

Definition 7.13 (Candidate transported lift). A *candidate transported lift* for the i -th transported chemical generator is a continuous path

$$\tilde{\gamma}_i^\Lambda : [0, 1] \longrightarrow \tilde{\mathcal{X}}_{p_i}^\Lambda \quad (439)$$

that:

1. has the chemically transported source and target;
2. respects the persistent local atom correspondence; and
3. is not yet assumed to satisfy every hard cage constraint.

Let

$$F_{ij}^\Lambda \quad (440)$$

denote the corresponding transported constraint functionals, indexed under the declared local correspondence.

Define

$$\Delta_{ij}^\Lambda := \sup_{t \in [0, 1]} \left| F_{ij}^\Lambda(\tilde{\gamma}_i^\Lambda(t)) - F_{ij}^{\Lambda_0}(\gamma_i(t)) \right| \quad (441)$$

and

$$\Delta_{\mathcal{F}}^\Lambda := \max_{i,j} \Delta_{ij}^\Lambda. \quad (442)$$

The quantity $\Delta_{\mathcal{F}}^\Lambda$ measures perturbation of the actual constraint values rather than requiring equality of the complete molecular geometries.

7.6 Persistence of cage admissibility

Theorem 7.14 (Persistence of cage admissibility for transported lifts). *Let $\mathbf{p}_C^{\Lambda_0}$ have uniform positive cage margin*

$$m_{\min} > 0. \quad (443)$$

Suppose that for another $\Lambda \in \mathcal{L}$:

1. *the corresponding chemical path has been transported;*
2. *a candidate transported lift $\tilde{\gamma}_i^\Lambda$ exists for every transported generator; and*
- 3.

$$\Delta_{\mathcal{F}}^\Lambda < m_{\min}. \quad (444)$$

Then every candidate transported lift satisfies every corresponding hard cage constraint. Consequently,

$$\tilde{\gamma}_i^\Lambda \in \text{Lift}_C(p_i^\Lambda; S_i^\Lambda, S_{i+1}^\Lambda) \quad (445)$$

for all i , and the transported chemical word defines a cage-constrained reaction path.

Proof. For every i, j and $t \in [0, 1]$,

$$F_{ij}^\Lambda(\tilde{\gamma}_i^\Lambda(t)) \leq F_{ij}^{\Lambda_0}(\gamma_i(t)) + \Delta_{\mathcal{F}}^\Lambda \quad (446)$$

$$\leq -m_{ij} + \Delta_{\mathcal{F}}^\Lambda \quad (447)$$

$$\leq -m_{\min} + \Delta_{\mathcal{F}}^\Lambda \quad (448)$$

$$< 0. \quad (449)$$

Thus every candidate transported path remains strictly inside every designated hard transition constraint. Its endpoints likewise satisfy the corresponding state constraints. Hence each candidate path is a geometric lift of its transported chemical rewrite. Finite composition gives the transported cage-constrained path. $\square$

Remark 7.15 (Scope of the persistence theorem). Theorem 7.14 proves persistence of *admissibility* for a supplied candidate geometric transport. Existence of that candidate transport is a separate realization condition and is not inferred from the positive-margin argument.

7.7 Coordinate-space sufficient condition

For computational comparison, geometric proximity may be easier to measure than direct constraint deviation.

Fix a proper-Euclidean gauge on the common finite cage support C . For corresponding configurations define

$$d_{SE(3)}(x, \tilde{x}) := \inf_{g \in SE(3)} \max_{a \in C} \|x(a) - g\tilde{x}(a)\|_2. \quad (450)$$

Assume that on a neighborhood of the reference lifts there exists a modulus

$$\omega : [0, \infty) \longrightarrow [0, \infty) \quad (451)$$

satisfying

$$\lim_{\varepsilon \rightarrow 0} \omega(\varepsilon) = 0 \quad (452)$$

and such that

$$\sup_i \sup_t d_{SE(3)}(\gamma_i(t), \tilde{\gamma}_i^\Lambda(t)) < \varepsilon \quad (453)$$

implies

$$\Delta_{\mathcal{F}}^\Lambda \leq \omega(\varepsilon). \quad (454)$$

Corollary 7.16 (Coordinate-space persistence radius). Under the preceding continuity condition, there exists

$$\varepsilon_0 > 0 \quad (455)$$

such that every already defined family of candidate transported lifts satisfying

$$\sup_i \sup_{t \in [0, 1]} d_{SE(3)}(\gamma_i(t), \tilde{\gamma}_i^\Lambda(t)) < \varepsilon_0 \quad (456)$$

also satisfies

$$\Delta_{\mathcal{F}}^\Lambda < m_{\min}. \quad (457)$$

Hence the candidate transports are cage admissible by Theorem 7.14.

Proof. Choose $\varepsilon_0 > 0$ such that

$$\omega(\varepsilon_0) < m_{\min}. \quad (458)$$

Then Equation (454) gives

$$\Delta_{\mathcal{F}}^\Lambda < m_{\min},$$

and the preceding theorem applies. $\square$

Thus ε_0 is a persistence radius for the *admissibility* of corresponding candidate transports. It is not an existence theorem for those transports.

7.8 Local transformation invariance over the substitution family

Definition 7.17 (Local transformation invariance). A cage-constrained reaction word is *locally transformation invariant* over $\mathcal{L}$ when, for every $\Lambda \in \mathcal{L}$, there exists a corresponding cage-constrained path having:

1. the same ordered transported local rewrite word; and
2. the same principal terminal restriction under the canonical local atom identification.

Theorem 7.18 (Local transformation invariance over the substitution family). Let

$$\Lambda_0 \in \mathcal{L} \quad (459)$$

and suppose there exists a reference path

$$\mathbf{p}_C^{\Lambda_0} : S_0^{\Lambda_0} \rightsquigarrow_C^* T^{\Lambda_0} \quad (460)$$

whose chemical support is contained in U_{rxn} .

Assume:

1. Hypothesis 7.8 holds throughout $\mathcal{L}$;
2. every external substitution context is reaction inert relative to the reference path grammar;
3. the selected reference lifts possess uniform positive cage margin

$$m_{\min} > 0; \quad (461)$$

4. for every $\Lambda \in \mathcal{L}$, every chemically transported generator possesses a candidate transported lift; and
5. those candidate lifts satisfy

$$\Delta_{\mathcal{F}}^{\Lambda} < m_{\min}. \quad (462)$$

Then for every

$$\Lambda \in \mathcal{L} \quad (463)$$

there exists a cage-constrained path

$$\mathbf{p}_C^{\Lambda} : S_0^{\Lambda} \rightsquigarrow_C^* T^{\Lambda} \quad (464)$$

with

$$T^{\Lambda} \equiv_{U_{\text{rxn}}} T^{\Lambda_0}. \quad (465)$$

Hence the selected reaction word is locally transformation invariant over $\mathcal{L}$.

Proof. Theorem 7.6 transports the ordered chemical rewrite word to every substitution context.

For each transported word, candidate geometric paths exist by hypothesis. Theorem 7.14 then promotes each candidate path to a geometric lift because its constraint deviation is smaller than the reference positive margin. The transported elementary transitions therefore compose in the cage-constrained reaction category. Local terminal equivalence follows from the exact chemical context-extension construction. $\square$

A sufficient computational form of assumption 5 is

$$\varepsilon_{\Lambda} < \varepsilon_0, \quad (466)$$

provided that the candidate transported lifts exist and the continuity condition of Corollary 7.16 holds.

7.9 Target-family consequence

Corollary 7.19 (Substitution-pattern invariance of target reachability). Assume the hypotheses of Theorem 7.18.

If

$$T^{\Lambda_0} \in \mathfrak{T}_{\star}^{\Lambda_0} \quad (467)$$

and the target predicate depends only on:

1. the locally preserved principal target motif;
2. the selected stereochemical label; and
3. independently admissible context-specific coproduct conditions,

then for every $\Lambda \in \mathcal{L}$ there exists

$$T^{\Lambda} \in \mathfrak{T}_{\star}^{\Lambda} \quad (468)$$

such that

$$\text{Hom}_{\mathbf{Reach}_{\Lambda}^{6 \rightarrow 5}}(S_0^{\Lambda}, T^{\Lambda}) \neq \emptyset. \quad (469)$$

Proof. Theorem 7.18 gives a transported cage-constrained path with the same local terminal restriction. The target predicate is therefore preserved on the principal product, while the remaining coproduct conditions hold by hypothesis. $\square$

7.10 Persistence of the selected stereochemical branch

Let

$$\zeta_{\chi}(t) := \langle u_{\text{att}}(t), e_3(t) \rangle \quad (470)$$

be the oriented attack observable used to distinguish the two local stereochemical branches.

Definition 7.20 (Robust stereochemical margin). A selected reference amino-installation lift has *stereochemical margin* $\delta_{\chi} > 0$ when

$$|\zeta_{\chi}(t)| \geq \delta_{\chi} \quad (471)$$

throughout the stereochemistry-determining portion of the lift.

Corollary 7.21 (Persistence of the selected stereochemical branch). Suppose:

1. the reference amino-installation rule is stereospecific with respect to the sign of ζ_{χ} ;
2. the selected reference lift produces $\chi_{\star}$ and has margin $\delta_{\chi} > 0$; and
3. a transported candidate amino-installation lift satisfies

$$\sup_t |\tilde{\zeta}_{\chi}(t) - \zeta_{\chi}(t)| < \delta_{\chi}. \quad (472)$$

Then the transported candidate lift retains the same

oriented attack sign and therefore produces

$$\chi(c_\alpha) = \chi_\star. \quad (473)$$

Proof. Equation (471) places the reference attack observable a positive distance from zero. Condition (472) therefore prevents the transported observable from changing sign. Stereospecificity of the local rewrite then preserves the same product configuration. $\square$

This corollary establishes persistence of the *selected transported stereochemical branch*. A stronger claim that the opposite branch is globally absent from the entire perturbed realization requires the corresponding strong cage-exclusion hypothesis separately.

7.11 Hierarchy and failure conditions

The resulting locality structure is:

$$\begin{array}{c}
 \text{exact local chemical concordance} \\
 \Downarrow \\
 \text{exact chemical path transport} \\
 \Downarrow \\
 \text{candidate geometric transport} \\
 \Downarrow \Delta_{\mathcal{F}} < m_{\min} \\
 \text{cage-admissible transported path} \\
 \Downarrow \delta_\chi > 0 \\
 \text{preserved selected stereochemical branch.}
 \end{array} \quad (474)$$

Local transformation invariance may therefore fail at distinct levels:

1. a modification enters U_{rxn} ;
2. local chemical concordance fails;
3. no corresponding candidate geometric transport exists;
4. the transported candidate crosses a hard cage boundary,

$$\Delta_{\mathcal{F}}^{\Delta} \geq m_{\min};$$

or

5. the selected stereochemical trajectory crosses

$$\zeta_\chi = 0.$$

For the three substitution contexts in $\mathcal{L}$, the chemical rewrite word is therefore transported exactly under Hypothesis 7.8, whereas cage-level and stereochemical persistence require the additional candidate-transport and positive-margin hypotheses.

The next section constructs the explicit $C6 \rightarrow C5$ reaction word to which these locality results are applied.

8 A Constructive Reference Path for the $C6 \rightarrow C5$ Realization

We now construct an explicit finite reaction word joining the reference saturated tether state to the principal target connectivity.

The purpose of the construction is to provide a witness candidate for the existence theorems of Section 9. The present section specifies:

$$\begin{array}{c}
 \text{persistent atom identities,} \\
 \Downarrow \\
 \text{six ordered local graph transformations,} \\
 \Downarrow \\
 \text{their atom-map and protected-invariant properties,} \\
 \Downarrow \\
 \text{the resulting canonical reaction word.}
 \end{array} \quad (475)$$

Chemical admissibility and cage liftability are imposed explicitly below as realization hypotheses. The complete balanced

$$L \longleftarrow K \longrightarrow R \quad (476)$$

representations of the six local rules are collected in Appendix B.

8.1 Persistent local atom identities

In addition to

$$v_5, v_6, o_6, c_\alpha, c_\beta, o_\beta, p, o_{2'}, \quad (477)$$

introduce:

$$o_x \quad (478)$$

as the oxygen atom that becomes the canonical C_β carbonyl oxygen, and

$$n_\alpha \quad (479)$$

as the nitrogen atom that becomes the amino nitrogen.

Let

$$h_5 \quad (480)$$

denote the hydrogen initially attached to v_5 .

The remaining mapped hydrogens on c_α , c_β , and $o_{2'}$ are retained in the closed reaction atom universe but are suppressed from most displayed skeletal formulas.

Convention 8.1 (Suppressed hydrogen and reagent bookkeeping). Every displayed local transformation in this section is the projection of a complete atom- and charge-balanced rule in the closed reaction universe. Thus a notation such as



means that the removed mapped hydrogen is transferred to an explicitly represented reagent or coproduct state. No atom is created or destroyed by the displayed shorthand.

8.2 Reference initial state

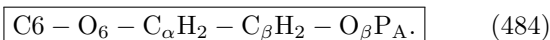
For

$$\Lambda \in \mathcal{L}, \quad (482)$$

the canonical initial state

$$S_0^\Lambda \quad (483)$$

contains the local motif



The target bonds are initially absent:

$$\bar{b}_{S_0}(v_5, c_\alpha) = 0, \quad \bar{b}_{S_0}(c_\beta, o_{2'}) = 0. \quad (485)$$

The inherited chrysene edge

$$\{v_5, v_6\} \quad (486)$$

belongs to the protected carbon framework and is preserved throughout the construction.

8.3 Canonical local generators

The canonical witness uses six ordered local generators. For each generator, only the net local atom-mapped transformation is given here. Appendix B provides the complete balanced rewrite data.

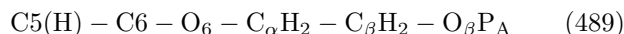
Capture generator. Define

$$p_{\text{cap}} : S_0^\Lambda \longrightarrow S_1^\Lambda \quad (487)$$

by the principal bond changes

$$\begin{aligned} \bar{b}(o_6, c_\alpha) &: 1 \mapsto 0, \\ \bar{b}(v_5, c_\alpha) &: 0 \mapsto 1, \\ \bar{b}(v_5, h_5) &: 1 \mapsto 0, \\ \bar{b}(o_6, h_5) &: 0 \mapsto 1. \end{aligned} \quad (488)$$

The projected local effect is



No chrysene carbon-carbon edge is altered.

Unsaturation generator. Define

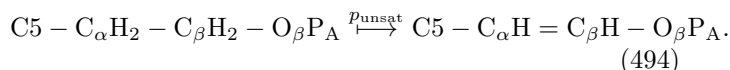
$$p_{\text{unsat}} : S_1^\Lambda \longrightarrow S_2^\Lambda \quad (492)$$

by increasing the $c_\alpha - c_\beta$ bond order

$$\bar{b}(c_\alpha, c_\beta) : 1 \mapsto 2 \quad (493)$$

and transferring one mapped hydrogen from each carbon to the explicitly represented hydrogen-accepting part of the closed reaction universe.

The projected effect is



Oxygen-addition generator. Let o_x be supplied by an explicitly represented oxygen-donor component.

Define

$$p_{\text{epox}} : S_2^\Lambda \longrightarrow S_3^\Lambda \quad (495)$$

by

$$\begin{aligned} \bar{b}(c_\alpha, c_\beta) &: 2 \mapsto 1, \\ \bar{b}(c_\alpha, o_x) &: 0 \mapsto 1, \\ \bar{b}(c_\beta, o_x) &: 0 \mapsto 1. \end{aligned} \quad (496)$$

The resulting local subgraph contains the three-membered cycle



while retaining



Carbonyl-forming generator. Define

$$p_{\text{carb}} : S_3^\Lambda \longrightarrow S_4^\Lambda \quad (499)$$

by the local changes

$$\begin{aligned} \bar{b}(c_\alpha, o_x) &: 1 \mapsto 0, \\ \bar{b}(c_\beta, o_x) &: 1 \mapsto 2, \end{aligned} \quad (500)$$

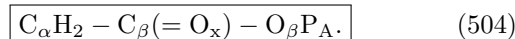
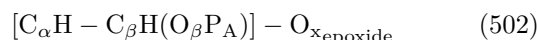
together with transfer of the mapped c_β hydrogen specified in Appendix A to c_α .

The bond

$$\bar{b}(c_\beta, o_\beta) = 1 \quad (501)$$

is retained.

The projected net effect is therefore



Amino-installation generator. Let n_α be supplied by an explicitly represented nitrogen-donor component.

Define

$$p_{\text{am}} : S_4^\Lambda \longrightarrow S_5^\Lambda \quad (505)$$

by replacing one mapped $c_\alpha - H$ bond with

$$\bar{b}(c_\alpha, n_\alpha) : 0 \longmapsto 1, \quad (506)$$

with the displaced hydrogen transferred to an allowed coproduct state.

The projected product contains

$$\boxed{\text{C5} - \text{C}_\alpha(\text{H})(\text{NH}_2) - \text{C}_\beta(=\text{O}_x) - \text{O}_\beta\text{P}_\text{A}}. \quad (507)$$

At this state the four substituent classes at c_α are distinct:

$$c_\alpha \sim (C5, C_\beta, \text{NH}_2, H). \quad (508)$$

Consequently, c_α admits an absolute stereochemical label

$$\chi(c_\alpha) \in \{R, S\}. \quad (509)$$

Terminal acyl-transfer generator. Define

$$p_{\text{tr}} : S_5^\Lambda \longrightarrow S_6^\Lambda \quad (510)$$

by

$$\begin{aligned} \bar{b}(c_\beta, o_\beta) : 1 &\longmapsto 0, \\ \bar{b}(c_\beta, o_{2'}) : 0 &\longmapsto 1, \end{aligned} \quad (511)$$

while retaining

$$\bar{b}(c_\beta, o_x) = 2. \quad (512)$$

The mapped proton initially associated with the 2'-hydroxyl is transferred into an admissible terminal phosphate-containing coproduct state.

The projected terminal transformation is

$$\text{C}_\beta(=\text{O}_x) - \text{O}_\beta\text{P}_\text{A} + \text{HO}_{2'}\text{Ado} \quad (513)$$

$$\xrightarrow{p_{\text{tr}}} \quad (514)$$

$$\text{C}_\beta(=\text{O}_x) - \text{O}_{2'}\text{Ado} + \text{Z}_P. \quad (515)$$

The complete atom-balanced terminal state is

$$S_6^\Lambda. \quad (516)$$

8.4 Canonical reaction word

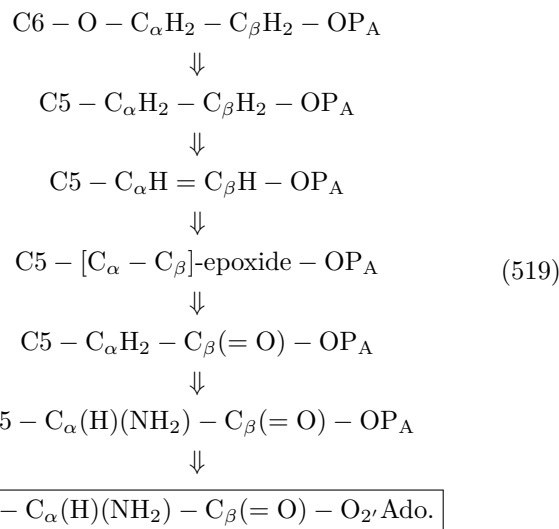
Define

$$\boxed{\Phi_{\text{can}} = p_{\text{tr}} \circ p_{\text{am}} \circ p_{\text{carb}} \circ p_{\text{epox}} \circ p_{\text{unsat}} \circ p_{\text{cap}}}. \quad (517)$$

Its state sequence is

$$\begin{aligned} S_0^\Lambda &\xrightarrow{p_{\text{cap}}} S_1^\Lambda \xrightarrow{p_{\text{unsat}}} S_2^\Lambda \\ &\xrightarrow{p_{\text{epox}}} S_3^\Lambda \xrightarrow{p_{\text{carb}}} S_4^\Lambda \\ &\xrightarrow{p_{\text{am}}} S_5^\Lambda \xrightarrow{p_{\text{tr}}} S_6^\Lambda. \end{aligned} \quad (518)$$

At the level of principal local motifs:



8.5 Atom-map and protected-invariant properties

Proposition 8.2 (Atom-map preservation). *Suppose each displayed generator is realized by its complete balanced rule in Appendix B. Then Φ_{can} is atom-map preserving.*

Proof. Every generator acts on the fixed persistent atom universe $\mathbb{A}$.

The capture rule moves the mapped hydrogen h_5 from v_5 to o_6 .

The unsaturation rule transfers mapped hydrogen atoms to explicitly represented acceptor or coproduct states.

The oxygen-addition rule transfers the pre-existing atom o_x from its donor component into the reactive subgraph.

The carbonyl-forming rule preserves o_x and converts its $c_\beta - o_x$ bond to the carbonyl double bond.

The amino-installation rule transfers the pre-existing atom n_α into the target subgraph.

The terminal transfer preserves $o_{2'}$, o_β , and the phosphate atoms while changing their connectivity.

Thus no atom identity, element label, or isotope label is created, destroyed, or exchanged. $\square$

Proposition 8.3 (Preservation of the chrysene molecular anchor). *The canonical reaction word preserves every inherited chrysene carbon-carbon edge and every chrysene locant identity. In particular,*

$$\bar{b}_{S_6}(v_5, v_6) = \bar{b}_{S_0}(v_5, v_6). \quad (520)$$

Proof. No generator changes a bond whose two endpoints are both chrysene carbon-framework vertices. The only new bond incident to the chrysene framework is

$$\{v_5, c_\alpha\}. \quad (521)$$

All inherited locant labels are unchanged. $\square$

Proposition 8.4 (Canonical carbonyl-oxygen provenance). *Under p_{epox} followed by p_{carb} , the carbonyl oxygen in S_4^Λ and all subsequent canonical states is the persistent atom o_x .*

$$o_{\text{carbonyl}} = o_x. \quad (522)$$

Proof. The oxygen-addition rule makes o_x a single-bonded neighbor of both c_α and c_β . The carbonyl-forming rule removes the $c_\alpha - o_x$ bond and increases the $c_\beta - o_x$ bond order from one to two. Subsequent canonical rules do not alter that double bond. $\square$

8.6 Locality of the canonical word

Let

$$\mathcal{P}_{\text{can}} = \{p_{\text{cap}}, p_{\text{unsat}}, p_{\text{epox}}, p_{\text{carb}}, p_{\text{am}}, p_{\text{tr}}\}. \quad (523)$$

By Definition 7.1, its completed local support is

$$U_{\text{rxn}} = U_6 \cup \bigcup_{p \in \mathcal{P}_{\text{can}}} \text{Pat}(p). \quad (524)$$

Hence

$$\text{Supp}(\Phi_{\text{can}}) \subseteq U_{\text{rxn}}. \quad (525)$$

Corollary 8.5 (Remote substitutions lie outside the canonical chemical support). *Suppose the additional C3, C9, and remote C12 decorations of the substitution family do not occur in the pattern support of $\mathcal{P}_{\text{can}}$. Then those decorations are reaction inert relative to the canonical chemical word.*

This is the chemical locality condition used by Section 7.

8.7 Admissibility packages for the canonical witness

The six displayed generators define a formal reaction word regardless of whether a particular physical realization satisfies the required chemical and geometric conditions. We therefore collect those conditions rather than restating an individual hypothesis after every generator.

Hypothesis 8.6 (Canonical chemical-admissibility package). For the selected reference realization:

1. every generator in $\mathcal{P}_{\text{can}}$ possesses a chemically admissible match;
2. every generator has a complete balanced realization in the closed reaction universe;
3. all resource-ledger updates remain admissible;
4. every rule application satisfies the global charge-balance condition of Section 4;
5. $\mathcal{I}_{\text{prot}}$ is preserved; and
6. the six rule applications are source-target composable in the order of Φ_{can} .

Hypothesis 8.7 (Canonical cage-lift package). For every canonical generator

$$p_i : S_{i-1}^\Lambda \longrightarrow S_i^\Lambda, \quad (526)$$

the corresponding lift space is nonempty:

$$\text{Lift}_C(p_i; S_{i-1}^\Lambda, S_i^\Lambda) \neq \emptyset. \quad (527)$$

Hypothesis 8.8 (Canonical stereochemical package). The amino-installation generator p_{am} is stereospecific with respect to the oriented attack sign σ_α , and its selected reference lift is strongly $\chi_\star$ -selective in the sense of Definition 5.6.

8.8 Chemical and cage-constrained witness

Theorem 8.9 (Conditional chemical validity of the canonical word). *Under Hypothesis 8.6,*

$$\Phi_{\text{can}} \in \text{Hom}_{\text{Chem}}(S_0^\Lambda, S_6^\Lambda). \quad (528)$$

Proof. Every generator is chemically admissible and the target of each generator is the source of the next. Their ordered composition is therefore a morphism in the free chemical path category. $\square$

Theorem 8.10 (Canonical cage-constrained witness). *Assume Hypotheses 8.6 and 8.7. Then*

$$\Phi_{\text{can}} \in \text{Hom}_{\text{Reach}_C}(S_0^\Lambda, S_6^\Lambda). \quad (529)$$

Equivalently,

$$S_0^\Lambda \preceq_C S_6^\Lambda. \quad (530)$$

Proof. Theorem 8.9 places all six generators in the chemical transition quiver.

Hypothesis 8.7 makes each generator cage liftable. They therefore belong to the generating quiver of $\mathbf{Reach}_C$, and their finite composition gives the claimed morphism. $\square$

Proposition 8.11 (Stereochemical refinement of the canonical witness). *Assume Hypothesis 8.8 in addition to the hypotheses of Theorem 8.10.*

Then

$$\chi_{S_5^\Lambda}(c_\alpha) = \chi_\star. \quad (531)$$

If p_{tr} does not alter any bond incident to c_α , then

$$\chi_{S_6^\Lambda}(c_\alpha) = \chi_\star. \quad (532)$$

Proof. The first conclusion follows from Proposition 5.7. The terminal transfer changes connectivity at c_β , o_β , and $o_{2'}$, but not at c_α . Hence the assigned configuration is preserved. $\square$

8.9 Principal target projection

Proposition 8.12 (Principal-product realization). *The principal-product projection of the canonical terminal state contains*

$$\mathcal{I}_{\text{conn}} = v_5 - c_\alpha(H)(NH_2) - c_\beta(=O_x) - o_{2'}. \quad (533)$$

Under Hypothesis 8.8, the corresponding stereochemical target motif is

$$\mathcal{I}_\star = [v_5 - c_\alpha(H)(NH_2) - c_\beta(=O_x) - o_{2'}]_{\chi_\star}. \quad (534)$$

Proof. The capture generator creates $\{v_5, c_\alpha\}$ and no later generator deletes it.

The amino-installation generator creates $\{c_\alpha, n_\alpha\}$.

The carbonyl-forming generator creates $\{c_\beta, o_x\}_2$, which is retained thereafter.

The terminal transfer creates $\{c_\beta, o_{2'}\}$.

The stereochemical statement follows from Proposition 8.11. $\square$

8.10 Composite carbonyl-generation morphism

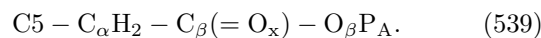
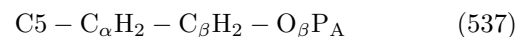
For comparison with alternative carbonyl-forming paths, define

$$P_\beta^{\text{epox}} := p_{\text{carb}} \circ p_{\text{epox}} \circ p_{\text{unsat}}. \quad (535)$$

Whenever the three generators are defined and composable,

$$P_\beta^{\text{epox}} : S_1^\Lambda \longrightarrow S_4^\Lambda \quad (536)$$

has the net local effect



The full canonical word may therefore be written

$$\Phi_{\text{can}} = p_{\text{tr}} \circ p_{\text{am}} \circ P_\beta^{\text{epox}} \circ p_{\text{cap}}. \quad (540)$$

Remark 8.13 (Composite versus elementary transformation). The symbol P_β^{epox} denotes a composite morphism, not an additional elementary generator. Its introduction therefore does not create a distinct reaction path merely by changing the level of description.

Alternative factorizations having the same source and target are treated in Section 10.

8.11 Constructive result

The canonical construction establishes the following conditional statement:

$$\begin{array}{c} \text{canonical chemical-admissibility package} \\ + \text{canonical cage-lift package} \\ \Downarrow \\ S_0^\Lambda \preceq_C S_6^\Lambda, \\ \pi_{\text{main}}(S_6^\Lambda) \supseteq \mathcal{I}_{\text{conn}}. \end{array} \quad (541)$$

With the additional stereochemical package,

$$\pi_{\text{main}}(S_6^\Lambda) \supseteq \mathcal{I}_\star. \quad (542)$$

The construction therefore supplies the explicit witness used by the reference and family-level existence theorems of Section 9. Physical certification of the individual generator hypotheses is treated separately in Section 11.

9 Cage-Constrained Transformation Existence

The preceding sections provide all ingredients required for a constructive reachability theorem:

$$\begin{array}{c}
 \text{typed atom-preserving chemical states} \\
 \Downarrow \\
 \text{chemically admissible local rewrites} \\
 \Downarrow \\
 \text{cage-liftable elementary transitions} \\
 \Downarrow \\
 \text{a finite constructive witness} \\
 \Downarrow \\
 \text{local transport across substitution contexts.}
 \end{array} \tag{543}$$

The present section collects the required hypotheses and proves, separately, connectivity-level existence, stereochemically specified existence, and family-level invariance.

Let

$$\mathcal{L} = \{\Lambda_2, \Lambda_3, \Lambda_4\} = \{\{6, 12\}, \{3, 6, 12\}, \{3, 6, 9, 12\}\}. \tag{544}$$

Fix initially one reference context

$$\Lambda_0 \in \mathcal{L}. \tag{545}$$

9.1 Reference hypothesis architecture

The canonical reaction word of Section 8 is

$$\Phi_{\text{can}} = p_{\text{tr}} \circ p_{\text{am}} \circ p_{\text{carb}} \circ p_{\text{epox}} \circ p_{\text{unsat}} \circ p_{\text{cap}}. \tag{546}$$

Rather than repeating the complete definition of every generator, we collect the assumptions needed by the existence theorem into five logically distinct packages.

Definition 9.1 (Structural hypothesis). The hypothesis H_{str} holds for the reference realization when:

1. the fixed chrysene molecular anchor and inherited locant data are present;
2. the initial state is the reference $C6 \rightarrow C5$, $C2$ -anchored realization $S_0^{\Lambda_0}$ of Section 3;
3. the ribose oxygen o_2 is available as the terminal $2'$ -oxygen acceptor before the transfer step; and
4. the protected invariant $\mathcal{I}_{\text{prot}}$ of Definition 4.19 is imposed throughout the path.

Definition 9.2 (Chemical hypothesis). The hypothesis H_{chem} holds when the six ordered rule applications in Φ_{can} :

1. possess chemically admissible matches;
2. are atom-map preserving;
3. satisfy the valence, resource, and global charge-conservation conditions of Section 4;
4. preserve $\mathcal{I}_{\text{prot}}$; and
5. are source–target composable in the displayed order.

Definition 9.3 (Cage-lift hypothesis). The hypothesis H_{C} holds when every elementary chemical transition in Φ_{can} has nonempty geometric lift space:

$$\text{Lift}_{\text{C}}(p_i; S_{i-1}^{\Lambda_0}, S_i^{\Lambda_0}) \neq \emptyset \tag{547}$$

for every generator p_i of the canonical word.

Definition 9.4 (Terminal bookkeeping hypothesis). The hypothesis H_{term} holds when the complete terminal state assigns:

$$o_6 \tag{548}$$

to an allowed state in $\mathcal{Z}_6$, all displaced mapped hydrogens to allowed states in $\mathcal{Z}_H$, and the departing phosphate-containing fragment to an allowed state in $\mathcal{Z}_P$, with complete atom, resource, and charge bookkeeping.

Definition 9.5 (Stereochemical hypothesis). The hypothesis H_{χ} holds when:

1. the amino-installation rule is stereospecific with respect to the oriented attack sign σ_{α} ;
2. its reference cage lift is strongly $\chi_{\star}$ -selective in the sense of Definition 5.6; and
3. the complete product substituent ordering defines

$$\kappa_{\alpha} : \{-1, +1\} \longrightarrow \{R, S\}, \tag{549}$$

so that the selected geometric branch corresponds to $\chi_{\star}$.

Define the connectivity-level reference package by logical conjunction:

$$\boxed{H_{\text{conn}} := H_{\text{str}} \wedge H_{\text{chem}} \wedge H_{\text{C}} \wedge H_{\text{term}}.} \tag{550}$$

The stereochemically specified reference package is

$$\boxed{H_{\text{ref}} := H_{\text{conn}} \wedge H_{\chi}.} \tag{551}$$

This formulation avoids treating hypothesis packages as set unions and makes the logical dependence explicit.

9.2 Connectivity and stereochemical target classes

Let

$$\mathfrak{T}_{\text{conn}}^{\Lambda} \quad (552)$$

denote the class of complete atom-balanced terminal states whose principal product contains

$$v_5 - c_{\alpha}(H)(NH_2) - c_{\beta}(=O) - o_{2'}, \quad (553)$$

without requiring a specified absolute configuration at c_{α} .

The stereochemically specified target class

$$\mathfrak{T}_{\star}^{\Lambda} \quad (554)$$

additionally requires

$$\chi(c_{\alpha}) = \chi_{\star}. \quad (555)$$

Hence

$$\mathfrak{T}_{\star}^{\Lambda} \subseteq \mathfrak{T}_{\text{conn}}^{\Lambda}. \quad (556)$$

9.3 Reference connectivity existence

Theorem 9.6 (Reference cage-constrained connectivity existence). *Fix $\Lambda_0 \in \mathcal{L}$ and assume H_{conn} . Then there exists*

$$T_{\text{conn}}^{\Lambda_0} \in \mathfrak{T}_{\text{conn}}^{\Lambda_0} \quad (557)$$

such that

$$\text{Hom}_{\text{Reach}_{\Lambda_0}^{6 \rightarrow 5}}(S_0^{\Lambda_0}, T_{\text{conn}}^{\Lambda_0}) \neq \emptyset. \quad (558)$$

Proof. By H_{chem} , the ordered generators of Φ_{can} form a well-defined chemically admissible reaction word.

By H_{C} , each generator possesses a geometric lift. Hence Φ_{can} defines a morphism

$$\Phi_{\text{can}} : S_0^{\Lambda_0} \longrightarrow S_6^{\Lambda_0} \quad (559)$$

in $\text{Reach}_{\Lambda_0}^{6 \rightarrow 5}$.

The canonical target construction of Section 8 gives the principal local connectivity

$$v_5 - c_{\alpha}(H)(NH_2) - c_{\beta}(=O) - o_{2'}. \quad (560)$$

The hypothesis H_{term} places all remaining mapped atoms in admissible terminal coproduct states. Therefore

$$S_6^{\Lambda_0} \in \mathfrak{T}_{\text{conn}}^{\Lambda_0}. \quad (561)$$

Taking

$$T_{\text{conn}}^{\Lambda_0} = S_6^{\Lambda_0} \quad (562)$$

proves the result. $\square$

9.4 Reference stereochemical existence

Theorem 9.7 (Reference stereochemical transformation existence). *Fix $\Lambda_0 \in \mathcal{L}$ and assume H_{ref} . Then there exists*

$$T_{\star}^{\Lambda_0} \in \mathfrak{T}_{\star}^{\Lambda_0} \quad (563)$$

such that

$$\text{Hom}_{\text{Reach}_{\Lambda_0}^{6 \rightarrow 5}}(S_0^{\Lambda_0}, T_{\star}^{\Lambda_0}) \neq \emptyset. \quad (564)$$

Moreover,

$$\chi_{T_{\star}^{\Lambda_0}}(c_{\alpha}) = \chi_{\star}. \quad (565)$$

Proof. Theorem 9.6 provides the canonical cage-constrained path through the amino-installation state. By H_{χ} and Proposition 5.7, the amino-installation step yields

$$\chi(c_{\alpha}) = \chi_{\star}. \quad (566)$$

The subsequent terminal transfer does not alter any bond incident to c_{α} , so the stereochemical label is preserved to the terminal state.

The terminal state therefore belongs to $\mathfrak{T}_{\star}^{\Lambda_0}$. $\square$

Corollary 9.8 (L-configured reference target). *Under the hypotheses of Theorem 9.7, suppose the complete stereochemical assignment of the realized product satisfies*

$$\chi_{\star} = \chi_L. \quad (567)$$

Then the reachable terminal target has the intended L-series configuration at c_{α} :

$$\chi(c_{\alpha}) = \chi_L. \quad (568)$$

The identification $\chi_{\star} = \chi_L$ is made only after the full product substituent ordering and the applicable L/D convention have been specified; no universal identification of L with S is assumed.

9.5 Family-level locality hypotheses

To transport a reference witness across $\mathcal{L}$, the revised locality theory of Section 7 requires both exact chemical transport and a separately supplied geometric candidate transport.

Definition 9.9 (Connectivity locality package). Let $H_{\text{loc}}^{\text{conn}}$ denote the conjunction of the following conditions.

- (L1) Hypothesis 7.8 holds throughout $\mathcal{L}$.
- (L2) Every external substitution context is reaction

inert relative to the canonical rule grammar.

- (L3) The selected reference lifts possess a uniform positive cage margin

$$m_{\min} > 0. \quad (569)$$

- (L4) For every $\Lambda \in \mathcal{L}$ and every chemically transported canonical generator, a candidate transported lift exists in the sense of Definition 7.13.

- (L5) Every candidate transported path satisfies

$$\Delta_{\mathcal{F}}^{\Lambda} < m_{\min}. \quad (570)$$

- (L6) The terminal coproduct predicate is preserved under the local transport: the transported o_6 , hydrogen, and phosphate-containing terminal fragments remain members of their declared admissible classes.

Condition (L5) may be replaced by the sufficient coordinate-space condition

$$\varepsilon_{\Lambda} < \varepsilon_0 \quad (571)$$

whenever the hypotheses of Corollary 7.16 hold.

Definition 9.10 (Stereochemical locality package). Define

$$H_{\text{loc}}^{\chi} := H_{\text{loc}}^{\text{conn}} \wedge H_{\text{trans}\chi}, \quad (572)$$

where $H_{\text{trans}\chi}$ is the condition that, for every transported amino-installation candidate lift,

$$\sup_t \left| \tilde{\zeta}_{\chi}(t) - \zeta_{\chi}(t) \right| < \delta_{\chi}. \quad (573)$$

By Corollary 7.21, this condition preserves the selected stereochemical branch.

Define the family-level packages

$$\begin{aligned} H_{\text{fam}}^{\text{conn}} &:= H_{\text{conn}} \wedge H_{\text{loc}}^{\text{conn}}, \\ H_{\text{fam}}^{\chi} &:= H_{\text{ref}} \wedge H_{\text{loc}}^{\chi}. \end{aligned} \quad (574)$$

9.6 Family-level connectivity existence

Theorem 9.11 (Family-level connectivity existence). Assume that for one reference context

$$\Lambda_0 \in \mathcal{L} \quad (575)$$

the connectivity package H_{conn} holds, and assume $H_{\text{loc}}^{\text{conn}}$ throughout $\mathcal{L}$.

Then for every

$$\Lambda \in \mathcal{L} \quad (576)$$

there exists

$$T_{\text{conn}}^{\Lambda} \in \mathfrak{T}_{\text{conn}}^{\Lambda} \quad (577)$$

such that

$$\text{Hom}_{\text{Reach}_{\Lambda}^{6 \rightarrow 5}}(S_0^{\Lambda}, T_{\text{conn}}^{\Lambda}) \neq \emptyset. \quad (578)$$

Proof. Theorem 9.6 supplies a reference cage-constrained witness

$$S_0^{\Lambda_0} \rightsquigarrow_{\mathcal{C}}^* T_{\text{conn}}^{\Lambda_0}. \quad (579)$$

Conditions (L1) and (L2) transport the ordered chemical word to every $\Lambda \in \mathcal{L}$ by Theorem 7.6.

Conditions (L3)–(L5) allow Theorem 7.14 to promote each supplied candidate geometric transport to a genuine cage lift.

Hence the transported generators compose to give a cage-constrained path in every substitution context.

The local terminal connectivity is preserved by Theorem 7.18, and condition (L6) supplies the required terminal coproduct bookkeeping. Therefore the transported terminal state belongs to $\mathfrak{T}_{\text{conn}}^{\Lambda}$. $\square$

9.7 Main stereochemical existence theorem

Theorem 9.12 (Cage-Constrained Transformation Existence Theorem). Assume that there exists a reference substitution context

$$\Lambda_0 \in \mathcal{L} \quad (580)$$

for which H_{ref} holds, and assume H_{loc}^{χ} throughout $\mathcal{L}$. Then

$$\begin{aligned} &\forall \Lambda \in \mathcal{L}, \\ &\exists T_{\star}^{\Lambda} \in \mathfrak{T}_{\star}^{\Lambda} \quad \text{such that} \\ &\text{Hom}_{\text{Reach}_{\Lambda}^{6 \rightarrow 5}}(S_0^{\Lambda}, T_{\star}^{\Lambda}) \neq \emptyset, \\ &\chi_{T_{\star}^{\Lambda}}(c_{\alpha}) = \chi_{\star}. \end{aligned} \quad (581)$$

Proof. Theorem 9.7 provides a reference cage-constrained witness with

$$\chi(c_{\alpha}) = \chi_{\star}. \quad (582)$$

The connectivity part of H_{loc}^{χ} satisfies the hypotheses of Theorem 7.18. Hence the same ordered local reaction word is represented by a cage-constrained path in every $\Lambda \in \mathcal{L}$.

The additional stereochemical transport condition

$$\sup_t \left| \tilde{\zeta}_{\chi}(t) - \zeta_{\chi}(t) \right| < \delta_{\chi} \quad (583)$$

allows Corollary 7.21 to preserve the selected branch:

$$\chi(c_\alpha) = \chi_\star. \quad (584)$$

The locally preserved target connectivity together with the transported terminal bookkeeping condition places the terminal state in $\mathfrak{T}_\star^\Lambda$.

Therefore the stated hom-set is nonempty for every $\Lambda \in \mathcal{L}$. $\square$

Corollary 9.13 (Family-level L-configured target existence). *Assume Theorem 9.12 and suppose*

$$\chi_\star = \chi_L. \quad (585)$$

Then for every $\Lambda \in \mathcal{L}$ there exists a reachable terminal state

$$T_L^\Lambda \in \mathfrak{T}_\star^\Lambda \quad (586)$$

with

$$\chi_{T_L^\Lambda}(c_\alpha) = \chi_L. \quad (587)$$

9.8 Structural and atom-provenance consequences

Every canonical terminal witness supplied by the preceding theorems contains the local relations

$$\begin{aligned} \bar{b}(v_5, c_\alpha) &= 1, \\ \bar{b}(c_\alpha, c_\beta) &= 1, \\ \bar{b}(c_\alpha, n_\alpha) &= 1, \\ \bar{b}(c_\beta, o_x) &= 2, \\ \bar{b}(c_\beta, o_{2'}) &= 1. \end{aligned} \quad (588)$$

At the same time,

$$\bar{b}(v_5, v_6) = \bar{b}_{G_{\text{chr}}}(v_5, v_6), \quad (589)$$

so the inherited $C5 - C6$ chrysene carbon-framework edge is preserved.

Corollary 9.14 (No chrysene-ring scission in the canonical witness). *Formation of the canonical target $C5 - C_\alpha$ bond does not require cleavage of the inherited $C5 - C6$ carbon-carbon edge.*

For the canonical oxygenation/carbonyl factorization, persistent atom mapping additionally gives:

Corollary 9.15 (Canonical carbonyl-oxygen provenance). *For the canonical witness,*

$$o_{\text{carbonyl}} = o_x. \quad (590)$$

The original tether oxygen o_6 is not the C_β carbonyl oxygen in this factorization.

This provenance conclusion is path specific. Alternative admissible factorizations considered later may carry a different oxygen-provenance map.

9.9 Scope of the existence result

The preceding results establish nonempty conditional reachability:

$$\text{Hom}(S_0^\Lambda, T_\star^\Lambda) \neq \emptyset. \quad (591)$$

They do not require uniqueness or energetic optimality of the witness. Alternative reaction words are treated in Section 10, while physical instantiation of the chemical, geometric, and stereochemical hypotheses is addressed by the certification framework of Section 11.

9.10 Compressed theorem form

For later citation, the principal result is:

$$\begin{aligned} & H_{\text{ref}} \wedge H_{\text{loc}}^\chi \\ & \Downarrow \\ & \forall \Lambda \in \{\{6, 12\}, \{3, 6, 12\}, \{3, 6, 9, 12\}\}, \\ & \quad \exists T_\star^\Lambda \in \mathfrak{T}_\star^\Lambda \\ & \quad \text{with} \\ & \quad \text{Hom}_{\text{Reach}_\Lambda^{6 \rightarrow 5}}(S_0^\Lambda, T_\star^\Lambda) \neq \emptyset, \\ & \quad \chi_{T_\star^\Lambda}(c_\alpha) = \chi_\star. \end{aligned} \quad (592)$$

At the weaker connectivity level,

$$\begin{aligned} & H_{\text{conn}} \wedge H_{\text{loc}}^{\text{conn}} \\ & \Downarrow \\ & \forall \Lambda \in \mathcal{L}, \quad \exists T_{\text{conn}}^\Lambda \in \mathfrak{T}_{\text{conn}}^\Lambda \\ & \quad \text{with} \\ & \quad \text{Hom}_{\text{Reach}_\Lambda^{6 \rightarrow 5}}(S_0^\Lambda, T_{\text{conn}}^\Lambda) \neq \emptyset. \end{aligned} \quad (593)$$

Thus stereochemically specified existence is a strengthening of, and not a prerequisite for, connectivity-level reachability.

The next section examines alternative molecular realizations and distinct reaction words capable of reaching the same target class.

10 Alternative Realizations, Dual-Cipher Transport, and Reaction-Word Nonuniqueness

The existence theorem of Section 9 requires only one target-reaching morphism. The canonical witness of Section 8 provides such a morphism, but neither the reaction word nor the molecular realization need be unique.

Three distinct forms of nonuniqueness are relevant:

$$\begin{aligned} &\text{reaction-word nonuniqueness,} \\ &\text{molecular-realization nonuniqueness,} \\ &\text{terminal-coproduct nonuniqueness.} \end{aligned} \quad (594)$$

The first concerns distinct morphisms in the declared free reaction category. The second concerns distinct realization parameters whose associated reaction categories contain target-reaching paths. The third permits different complete atom-balanced terminal states to share the same principal molecular product.

These notions are treated separately below.

10.1 Reaction-word distinction and principal-product equivalence

Recall from Definition 6.12 that

$$\# \text{Hom}_{\text{Reach}_c}(S, T) \geq 2 \quad (595)$$

means that at least two distinct ordered elementary-transition words connect the same source and target.

This is a statement about the declared reaction grammar. A selected geometric lift is not itself part of the morphism datum.

Different complete terminal states may nevertheless encode the same principal product.

Definition 10.1 (Principal-product equivalence). Two complete terminal states T_1 and T_2 are *principal-product equivalent*, written

$$T_1 \sim_{\text{prod}} T_2, \quad (596)$$

when

$$\pi_{\text{main}}(T_1) = \pi_{\text{main}}(T_2) \quad (597)$$

as persistent-atom-labeled product graphs and, when stereochemistry is part of the target predicate,

$$\chi_{T_1}(c_\alpha) = \chi_{T_2}(c_\alpha). \quad (598)$$

Thus two terminal states may differ in phosphate, hydrogen, protonation, redox, or other coproduct data while representing the same principal target molecule.

Definition 10.2 (Product-class reaction-word nonuniqueness). A principal target product is *reaction-word nonunique relative to S* when there exist

$$T_1 \sim_{\text{prod}} T_2 \quad (599)$$

and reaction-word-distinct morphisms

$$f : S \longrightarrow T_1, \quad g : S \longrightarrow T_2. \quad (600)$$

Same-endpoint reaction-word nonuniqueness is therefore a special case of product-class reaction-word nonuniqueness.

10.2 Alternative factorizations of the C_β -carbonyl transformation

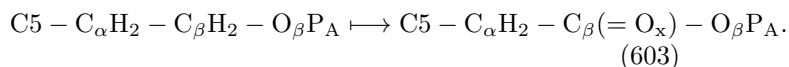
The canonical witness uses the composite

$$P_\beta^{\text{epox}} = p_{\text{carb}} \circ p_{\text{epox}} \circ p_{\text{unsat}}, \quad (601)$$

with source and target

$$P_\beta^{\text{epox}} : S_1 \longrightarrow S_4. \quad (602)$$

Its net local transformation is

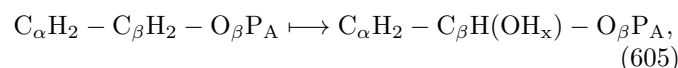


The reachability result depends on existence of a suitable morphism between these endpoint states, rather than on this factorization being the only possible one.

Hydroxylation–oxidation factorization. Let

$$q_{\text{hyd}} : S_1 \longrightarrow \tilde{S}_2 \quad (604)$$

be a local oxygenation rule with projected net effect

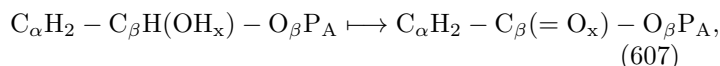


where the oxygen atom o_x is supplied by an explicitly represented oxygen donor.

Let

$$q_{\text{ox}} : \tilde{S}_2 \longrightarrow S_4 \quad (606)$$

have projected net effect



with removed hydrogen and redox equivalents transferred to declared states of the closed reaction universe.

Define

$$P_\beta^{\text{hyd}} := q_{\text{ox}} \circ q_{\text{hyd}}. \quad (608)$$

Hypothesis 10.3 (Hydroxylation–oxidation carbonyl route). The rules q_{hyd} and q_{ox} :

1. possess chemically admissible, atom-map-preserving balanced realizations;
2. preserve the protected chrysene anchor and the required $C_\beta - O_\beta - P_A$ linkage; and
3. are cage liftable:

$$\text{Lift}_C(q_{\text{hyd}}; S_1, \tilde{S}_2) \neq \emptyset, \quad (609)$$

$$\text{Lift}_C(q_{\text{ox}}; \tilde{S}_2, S_4) \neq \emptyset. \quad (610)$$

Under this hypothesis,

$$P_\beta^{\text{hyd}} \in \text{Hom}_{\text{Reach}_C}(S_1, S_4). \quad (611)$$

10.3 Two reaction words to the same terminal state

Suppose both

$$P_\beta^{\text{epox}}, \quad P_\beta^{\text{hyd}} \quad (612)$$

exist as cage-constrained morphisms from S_1 to S_4 .

Because their ordered generator words differ,

$$P_\beta^{\text{epox}} \neq P_\beta^{\text{hyd}} \quad (613)$$

in the free reaction category.

Theorem 10.4 (Reaction-word nonuniqueness from alternative carbonyl factorizations). *Assume:*

1. $P_\beta^{\text{epox}} : S_1 \rightarrow S_4$ exists;
2. $P_\beta^{\text{hyd}} : S_1 \rightarrow S_4$ exists;
3. the same capture morphism

$$p_{\text{cap}} : S_0 \rightarrow S_1$$

is available; and

4. the same downstream morphisms

$$p_{\text{am}} : S_4 \rightarrow S_5, \quad p_{\text{tr}} : S_5 \rightarrow S_6$$

are available.

Then the two composites

$$\Phi_{\text{epox}} = p_{\text{tr}} \circ p_{\text{am}} \circ P_\beta^{\text{epox}} \circ p_{\text{cap}} \quad (614)$$

and

$$\Phi_{\text{hyd}} = p_{\text{tr}} \circ p_{\text{am}} \circ P_\beta^{\text{hyd}} \circ p_{\text{cap}} \quad (615)$$

are distinct morphisms

$$\Phi_{\text{epox}}, \Phi_{\text{hyd}} : S_0 \rightarrow S_6. \quad (616)$$

Consequently,

$$\# \text{Hom}_{\text{Reach}_C}(S_0, S_6) \geq 2. \quad (617)$$

Proof. Both composites are defined by source–target compatibility.

Equality of morphisms in the free reaction category would require equality of their ordered elementary-transition words. Their middle subwords P_β^{epox} and P_β^{hyd} are distinct. Hence

$$\Phi_{\text{epox}} \neq \Phi_{\text{hyd}}.$$

□

Thus loss of one carbonyl factorization need not remove target reachability if the other remains available.

10.4 Atom provenance and stereochemical outcomes of alternative paths

Persistent atom mapping permits reaction-word-distinct paths to retain different experimentally testable information even when their principal unlabeled products agree.

For a morphism

$$f : S_0 \rightarrow T, \quad (618)$$

let

$$\text{Prov}_f : V(T) \rightarrow V(S_0) \cup V(\text{reagents}) \quad (619)$$

denote the atom-provenance map induced by persistent atom identity.

For the canonical epoxide-mediated path,

$$\text{Prov}_{\Phi_{\text{epox}}}(o_{\text{carbonyl}}) = o_x. \quad (620)$$

Another admissible path may, in principle, carry a different explicitly specified oxygen-provenance assignment.

Hence product-equivalent paths f and g may satisfy

$$\pi_{\text{main}}(T_f) = \pi_{\text{main}}(T_g) \quad (621)$$

while

$$\text{Prov}_f(o_{\text{carbonyl}}) \neq \text{Prov}_g(o_{\text{carbonyl}}). \quad (622)$$

Such a distinction is, in principle, accessible to isotope-labeling experiments and is incorporated into the certification framework of Section 11.

Reaction-word nonuniqueness also need not imply stereochemical nonuniqueness. Two distinct paths may satisfy

$$f \neq g \quad (623)$$

while

$$\chi_{T_f}(c_\alpha) = \chi_{T_g}(c_\alpha) = \chi_\star. \quad (624)$$

Conversely, distinct admissible paths may reach different stereochemical target classes.

For a target family $\mathfrak{T}$, define

$$\text{Hom}^{\chi_\star}(S, \mathfrak{T}) := \{f : S \rightarrow T : T \in \mathfrak{T}, \chi_T(c_\alpha) = \chi_\star\}. \quad (625)$$

The stereochemically specified existence condition is therefore

$$\text{Hom}^{\chi^*}(S, \mathfrak{T}) \neq \emptyset. \quad (626)$$

Exclusion of every opposite-configured target is a stronger statement and requires corresponding stereochemical hypotheses.

10.5 The dual-cipher $C5 \rightarrow C6$ realization

We next consider the paired local architecture obtained by exchanging the source and capture roles of the distinguished $C6/C5$ locants.

The reference realization is

$$C6 \longrightarrow C5, \quad (627)$$

whereas the dual realization is

$$C5 \longrightarrow C6. \quad (628)$$

Let

$$U_{\text{rxn}}^{6 \rightarrow 5} \quad (629)$$

be the completed local support of the reference grammar and let

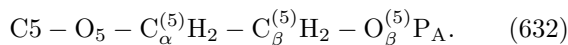
$$U_{\text{rxn}}^{5 \rightarrow 6} \quad (630)$$

be the corresponding dual support.

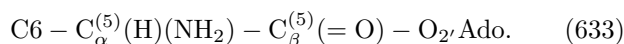
Introduce persistent dual tether labels

$$c_{\alpha}^{(5)}, \quad c_{\beta}^{(5)}, \quad o_5, \quad o_{\beta}^{(5)}, \quad (631)$$

with initial local motif



The corresponding principal target motif is



The inherited chrysene $C5 - C6$ edge remains protected.

10.6 Dual-cipher support transport and equivariance

Define the local support identification

$$\Sigma_{56} : U_{\text{rxn}}^{6 \rightarrow 5} \longrightarrow U_{\text{rxn}}^{5 \rightarrow 6} \quad (634)$$

on the principal persistent labels by

$$\begin{aligned} \Sigma_{56}(v_6) &= v_5, & \Sigma_{56}(v_5) &= v_6, \\ \Sigma_{56}(o_6) &= o_5, & \Sigma_{56}(c_{\alpha}) &= c_{\alpha}^{(5)}, \\ \Sigma_{56}(c_{\beta}) &= c_{\beta}^{(5)}, & \Sigma_{56}(o_{\beta}) &= o_{\beta}^{(5)}. \end{aligned} \quad (635)$$

Shared adenosine-side persistent atoms are fixed by Σ_{56} unless the selected dual realization explicitly specifies otherwise.

The map Σ_{56} is a labeled reaction-support identification. It is not assumed to arise from a proper or improper Euclidean symmetry of the instantiated molecule.

Definition 10.5 (Dual-cipher-equivariant reaction grammar). The reference local grammar $\mathcal{P}_{6 \rightarrow 5}$ is *dual-cipher equivariant* when

$$p \in \mathcal{P}_{6 \rightarrow 5} \implies (\Sigma_{56})_* p \in \mathcal{P}_{5 \rightarrow 6}. \quad (636)$$

Write the transported canonical generators as

$$p_{\text{cap}}^{(5)}, \quad p_{\text{unsat}}^{(5)}, \quad p_{\text{epox}}^{(5)}, \quad p_{\text{carb}}^{(5)}, \quad p_{\text{am}}^{(5)}, \quad p_{\text{tr}}^{(5)}. \quad (637)$$

The corresponding formal word is

$$\Phi_{\text{can}}^{5 \rightarrow 6} = p_{\text{tr}}^{(5)} \circ p_{\text{am}}^{(5)} \circ p_{\text{carb}}^{(5)} \circ p_{\text{epox}}^{(5)} \circ p_{\text{unsat}}^{(5)} \circ p_{\text{cap}}^{(5)}. \quad (638)$$

Hypothesis 10.6 (Dual-cipher cage compatibility). Every reference elementary cage transition appearing in the selected local path is transported by Σ_{56} to an elementary cage transition of the dual realization. Equivalently, for each selected generator,

$$\text{Lift}_C(p; S, T) \neq \emptyset \quad (639)$$

implies

$$\text{Lift}_C^{5 \rightarrow 6}((\Sigma_{56})_* p; (\Sigma_{56})_* S, (\Sigma_{56})_* T) \neq \emptyset. \quad (640)$$

Theorem 10.7 (Dual-cipher transport of reachability). Assume:

1. the reference local grammar is dual-cipher equivariant;
2. the dual initial state is the Σ_{56} -transport of the reference local initial state;
3. Hypothesis 10.6 holds; and
4. the transported terminal state satisfies the corresponding target and terminal-bookkeeping predicates.

Then Σ_{56} extends to a functor

$$\boxed{\mathfrak{D}_{56} : \mathbf{Reach}_{\Lambda}^{6 \rightarrow 5} [U_{\text{rxn}}^{6 \rightarrow 5}] \longrightarrow \mathbf{Reach}_{\Lambda}^{5 \rightarrow 6} [U_{\text{rxn}}^{5 \rightarrow 6}]} \quad (641)$$

In particular,

$$S_0^{6 \rightarrow 5} \preceq_C T_{\star}^{6 \rightarrow 5} \quad (642)$$

implies

$$S_0^{5 \rightarrow 6} \preceq_C T_{\star}^{5 \rightarrow 6}. \quad (643)$$

Proof. Dual-cipher equivariance transports every local chemical generator. Hypothesis 10.6 makes each transported generator an elementary cage transition.

Proposition 6.15 therefore extends the generator assignment uniquely to the functor $\mathfrak{D}_{56}$. Applying the functor to a reference witness produces the transported dual witness. $\square$

The theorem is a transport result for the declared local reaction architecture. It does not impose equality of activation barriers, rate constants, or stereochemical discrimination between the two realizations.

10.7 Adenine-anchor transport

The reference architecture uses

$$\eta_A = C2. \quad (644)$$

We also consider the alternative

$$\eta_A = N6. \quad (645)$$

Let

$$\mathcal{A}_{\text{anchor}} = \{C2, N6\} \quad (646)$$

and write

$$S_0^{\Lambda, \eta} \quad (647)$$

for the corresponding initial state.

Hypothesis 10.8 (Anchor-external chemical support). Replacing

$$\eta_A = C2 \longrightarrow \eta_A = N6 \quad (648)$$

does not alter the local chemical restriction on U_{rxn} , and every changed adenine/linker atom or bond lies outside the pattern footprint of the canonical reaction grammar.

Proposition 10.9 (Exact chemical transport under anchor change). *Under Hypothesis 10.8, the canonical local chemical reaction word for the C2-anchored realization transports exactly to the N6-anchored realization.*

Proof. The two realizations are exactly chemically concordant on U_{rxn} , and their differences lie in reaction-inert external context. Apply Theorem 7.6. $\square$

Anchor change may nevertheless modify the cage geometry. Accordingly, geometric transport requires a separate hypothesis.

Hypothesis 10.10 (Anchor-cage transport). For every chemically transported canonical generator in the N6-anchored realization:

1. a candidate transported lift exists; and
2. its hard-constraint deviation from the selected C2-anchored reference lift satisfies

$$\Delta_{\mathcal{F}}^{N6} < m_{\min}. \quad (649)$$

Theorem 10.11 (Adenine-anchor transport of reachability). *Assume Hypotheses 10.8 and 10.10.*

If

$$S_0^{\Lambda, C2} \preceq_C T^{\Lambda, C2}, \quad (650)$$

through the selected local reaction word, then there exists a corresponding terminal state $T^{\Lambda, N6}$ such that

$$S_0^{\Lambda, N6} \preceq_C T^{\Lambda, N6}. \quad (651)$$

Proof. Exact transport of the chemical reaction word follows from Proposition 10.9.

The candidate geometric transports exist by Hypothesis 10.10. Their constraint deviations satisfy the positive-margin condition, so Theorem 7.14 promotes them to genuine cage lifts.

The transported elementary transitions therefore compose to give the required path. $\square$

Corollary 10.12 (Stereochemical persistence under anchor change). *Assume the hypotheses of Theorem 10.11 and suppose the transported amino-installation candidate lift satisfies*

$$\sup_t \left| \tilde{\zeta}_X(t) - \zeta_X(t) \right| < \delta_X. \quad (652)$$

If the reference path produces

$$\chi^{C2}(c_\alpha) = \chi_\star, \quad (653)$$

then the transported path satisfies

$$\chi^{N6}(c_\alpha) = \chi_\star. \quad (654)$$

Proof. Apply Corollary 7.21 to the transported amino-installation lift. $\square$

10.8 General local realization transport

The substitution, dual-cipher, and adenine-anchor constructions are instances of one local transport principle.

Let

$$\mathcal{R}, \tilde{\mathcal{R}} \quad (655)$$

be two molecular realizations with completed local reaction supports

$$U, \tilde{U}. \quad (656)$$

Suppose

$$\varphi : U \longrightarrow \tilde{U} \quad (657)$$

is a labeled support bijection.

Theorem 10.13 (General local realization transport). *Assume:*

1. the selected reaction grammar is equivariant under φ ;
2. the initial states correspond on the complete local chemical support;
3. all realization differences outside the local support are reaction inert;
4. every transported generator is cage compatible, either directly or by the candidate-transport persistence theorem of Section 7; and
5. the transported terminal state satisfies the corresponding target and bookkeeping predicates.

Then there exists a functor

$$\Phi_\varphi : \mathbf{Reach}_C^{\mathcal{R}}[U] \longrightarrow \mathbf{Reach}_C^{\tilde{\mathcal{R}}}[\tilde{U}] \quad (658)$$

and target reachability in $\mathcal{R}$ implies reachability of the transported target in $\tilde{\mathcal{R}}$.

Proof. The assumptions supply a source–target-compatible transport of every selected generating transition. Proposition 6.15 then extends the generator map uniquely to a functor. Applying the functor to a target-reaching witness yields the transported witness. $\square$

The three principal applications are

$$\begin{aligned} \text{remote substitution: } \varphi &= \text{id}_{U_{\text{rxn}}}, \\ \text{dual cipher: } \varphi &= \Sigma_{56}, \\ \text{anchor variation: } \varphi &= \text{id}_{U_{\text{rxn}}} \quad \text{on the chemical support.} \end{aligned} \quad (659)$$

10.9 Realization nonuniqueness

Let

$$\mathbf{p} = (\Lambda, \eta_A, \ell_{\text{source}}, \ell_{\text{capture}}, \dots) \quad (660)$$

denote a molecular realization parameter.

Define the reachable realization family

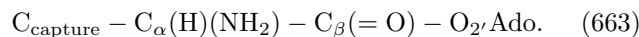
$$\mathcal{R}(T_\star) := \{\mathbf{p} : \exists T_\star^\mathbf{p} \text{ with } S_0^\mathbf{p} \preceq_C^\mathbf{p} T_\star^\mathbf{p}\}. \quad (661)$$

Definition 10.14 (Realization nonuniqueness). The target architecture is *realization nonunique* when

$$\#\mathcal{R}(T_\star) \geq 2. \quad (662)$$

For example, realization nonuniqueness occurs when two distinct admissible parameter values differ in source–capture orientation, adenine anchor, substitution context, or another declared realization parameter while both reach their corresponding target classes.

Across such realizations, the intended invariant is the target reaction topology



The following may vary:

$$\begin{aligned} &\text{source and capture locants,} \\ &\quad \text{adenine anchor,} \\ &\text{remote substitution context,} \\ &\quad \text{carbonyl factorization,} \\ &\quad \text{atom provenance,} \\ &\quad \text{cage geometry,} \\ &\quad \text{activation barriers,} \\ &\quad \text{stereochemical selectivity.} \end{aligned} \quad (664)$$

The existence problem is therefore naturally posed over a family of realizations rather than by requiring one uniquely specified microscopic construction.

10.10 Scope and transition to certification

The distinctions developed in this section are categorical and realization theoretic.

Reaction-word distinctness records different ordered rule/match words. A physical mechanistic interpretation additionally requires evidence that the corresponding chemical states, electronic pathways, and cage geometries are instantiated by the molecular system.

Likewise, a transported realization becomes a physical alternative only after its transport hypotheses have been certified.

The resulting structure is

$$\begin{array}{c} \boxed{\begin{array}{c} \text{one target-reaching witness} \\ \Downarrow \\ \text{target existence} \\ + \text{second reaction word} \\ \Downarrow \\ \text{reaction-word nonuniqueness} \\ + \text{second admissible realization} \\ \Downarrow \\ \text{realization nonuniqueness.} \end{array}} \end{array} \quad (665)$$

Detailed finite realization indexing, bounded path counts, length-minimal witnesses, path-cost functionals, and compatibility of multiple realization transports are collected in Appendix E.

The next section gives the computational and experimental certification framework needed to determine which reaction words and realization transports are physically instantiated.

11 Computational and Experimental Certification of the Realization Hypotheses

The existence theorems of Section 9 are conditional on explicitly declared realization hypotheses. The purpose of the present section is to define a finite certification framework for determining whether a specified molecular realization satisfies the hypotheses required by a selected theorem branch.

The logical relationship is

$$\begin{array}{c}
 \text{proved conditional theorem} \\
 H_{\Theta} \implies P \\
 \Downarrow \\
 \text{realization question} \\
 \text{Does a specified molecular system satisfy } H_{\Theta}? \\
 \Downarrow \\
 \text{computational and experimental certification.}
 \end{array} \quad (666)$$

Certification therefore tests the hypotheses of a theorem application; it does not alter the mathematical implication itself.

Detailed computational methods, experimental protocols, uncertainty models, ensemble criteria, and evidence matrices are collected in Appendix G.

11.1 Certification objects and status

Let

$$\mathcal{H} = \{H_1, \dots, H_N\} \quad (667)$$

be a finite family of realization hypotheses.

For each H_j , let

$$\mathcal{D}_j \quad (668)$$

be its declared evidence space and let

$$A_j : \mathcal{D}_j \longrightarrow \{0, 1\} \quad (669)$$

be a prospectively specified acceptance predicate.

Definition 11.1 (Realization certificate). A *realization certificate* for H_j is a tuple

$$\mathcal{C}_j = (H_j, M_j, D_j, A_j, R_j), \quad (670)$$

where:

1. M_j specifies the computational or experimental method;
2. $D_j \in \mathcal{D}_j$ is the resulting evidence object;
3. A_j is the declared acceptance predicate; and

4. R_j records resolution, uncertainty, domain of validity, and relevant methodological limitations.

The certificate is valid when

$$A_j(D_j) = 1. \quad (671)$$

A numerical result or molecular structure is therefore not, by itself, a certificate; it must be interpreted relative to a predefined criterion.

Define the certification-status set

$$\mathcal{V}_{\text{cert}} = \{U, C, F\}, \quad (672)$$

where

U = uncertified,

C = certified relative to the declared criterion, (673)

F = falsified relative to the declared criterion.

For each hypothesis,

$$\nu(H_j) \in \mathcal{V}_{\text{cert}}. \quad (674)$$

A status F means that the declared realization has failed the stated criterion for that hypothesis. It need not imply impossibility of every chemically distinct route to the same target.

11.2 Gate architecture for the canonical witness

The constructive path of Section 8 induces the canonical certification sequence

$$G_0 \longrightarrow G_1 \longrightarrow G_2 \longrightarrow G_3 \longrightarrow G_4 \longrightarrow G_5 \longrightarrow G_6 \longrightarrow G_7. \quad (675)$$

The gates have the following roles:

Gate	Certification target
G_0	Reference molecular structure and nonempty required cage domain.
G_1	$C6 \rightarrow C5$ capture compatible with the declared p_{cap} realization.
G_2	Atom-balanced $C_{\alpha} - C_{\beta}$ unsaturation.
G_3	Transfer of the mapped oxygen o_x to the declared oxygenated intermediate.
G_4	Formation of $C_{\beta} = O_x$ with retention of the required $C_{\beta} - O_{\beta} - P_A$ linkage.
G_5	Atom-balanced installation of n_{α} at C_{α} .
G_6	Stereochemical selection of $\chi_{\star}$.
G_7	Formation of the terminal $C_{\beta} - O_{2'}$ bond with admissible phosphate coproduct bookkeeping.

The gate order records the dependency structure of the canonical witness. It does not require that every formal intermediate be experimentally isolable.

11.3 Certification predicates for the principal gates

The detailed methods by which evidence is generated are realization specific. At the theorem interface, only the gate predicates are required.

Gate G_0 : structural and cage realization. Let

$$\mathcal{E}_0 = \{x_1, \dots, x_M\} \quad (676)$$

be a declared conformational ensemble for the initial realization.

The minimal existence-level criterion is

$$\exists x \in \mathcal{E}_0 \text{ such that } x \in \mathcal{K}(S_0). \quad (677)$$

A stronger realization may additionally require a prospectively specified ensemble population threshold. The precise sampling and uncertainty protocol is given in Appendix G.

Gate G_1 : $C_5 - C_\alpha$ capture. Gate G_1 requires evidence supporting the chemically balanced realization of

$$p_{\text{cap}} : S_0 \longrightarrow S_1 \quad (678)$$

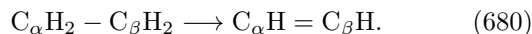
together with a compatible capture geometry and an accessible electronic pathway for the declared realization.

In particular, the evidence must support the mapped connectivity change

$$\bar{b}(v_5, c_\alpha) : 0 \longmapsto 1 \quad (679)$$

without destruction of the protected chrysene framework.

Gate G_2 : local unsaturation. Gate G_2 requires an atom-, resource-, and charge-balanced realization of



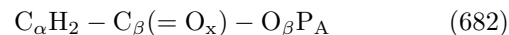
The mapped hydrogen atoms must terminate in explicitly represented acceptor or coproduct states.

Gate G_3 : oxygen addition. Gate G_3 requires an explicit oxygen-donor realization for which the persistent atom o_x is transferred to the declared oxygenated C_α/C_β intermediate:

$$\text{Prov}(o_{\text{oxygenated}}) = o_x. \quad (681)$$

Competing oxidation channels are evaluated according to prospectively specified selectivity criteria.

Gate G_4 : carbonyl formation with linkage retention. The canonical carbonyl gate requires an atom-map-resolved path to



while retaining the $C_\beta - \text{O}_\beta - \text{P}_A$ architecture required by the canonical witness.

Define

$$R_P = \begin{cases} 1, & \text{the certified path retains } C_\beta - \text{O}_\beta - \text{P}_A, \\ 0, & \text{otherwise.} \end{cases} \quad (683)$$

The canonical gate requires

$$R_P = 1. \quad (684)$$

Gate G_5 : amino installation. Gate G_5 requires an atom-balanced nitrogen-transfer realization forming

$$\bar{b}(c_\alpha, n_\alpha) = 1 \quad (685)$$

while preserving the protected chrysene anchor and the required C_β -carbonyl-containing architecture.

This gate certifies amino connectivity. Stereochemical selection is treated separately at G_6 .

Gate G_6 : stereochemical selection. The strong geometric gate is passed when the realized cage satisfies the condition of Definition 5.6:

$$\mathcal{U}_N \cap \mathcal{A}_{\chi_\star} \neq \emptyset, \quad \mathcal{U}_N \cap \mathcal{A}_{\chi_{\text{opp}}} = \emptyset. \quad (686)$$

This supports the deterministic conclusion

$$\chi(c_\alpha) = \chi_\star. \quad (687)$$

A distinct energetic gate may instead use

$$\Delta\Delta G_\chi^\ddagger = \Delta G_{\text{opp}}^\ddagger - \Delta G_\star^\ddagger \quad (688)$$

with a prospectively specified threshold. That gate supports a preferential rather than absolute stereochemical conclusion.

Gate G_7 : terminal 2'-O acyl transfer. Gate G_7 requires an atom-map-resolved transformation producing

$$\bar{b}(c_\beta, o_{2'}) = 1, \quad (689)$$

while:

1. retaining the $C_\beta = \text{O}$ bond;
2. assigning the phosphate-containing fragment to an allowed member of $\mathcal{Z}_P$;
3. preserving the target 2'-oxygen atom identity; and
4. satisfying the declared selectivity criterion against competing transfer modes.

11.4 Alternative carbonyl branch and certification fronts

The existence theory permits a second carbonyl-forming factorization

$$P_{\beta}^{\text{hyd}} = q_{\text{ox}} \circ q_{\text{hyd}}, \quad (690)$$

developed in Section 10.

Define the corresponding certification gate

$$G'_4 \quad (691)$$

to certify the complete $S_1 \rightarrow S_4$ hydroxylation–oxidation branch, including:

1. formation of the mapped C_{β} -hydroxylated intermediate;
2. retention of the required phosphate linkage;
3. oxidation to $C_{\beta} = O$; and
4. admissible atom, charge, and resource bookkeeping.

The two carbonyl routes therefore define different certificate sets.

For the canonical connectivity witness, let

$$\mathcal{G}_{\text{epox}}^{\text{conn}} = \{G_0, G_1, G_2, G_3, G_4, G_5, G_7\}. \quad (692)$$

For the alternative carbonyl branch, define

$$\mathcal{G}_{\text{hyd}}^{\text{conn}} = \{G_0, G_1, G'_4, G_5, G_7\}. \quad (693)$$

For stereochemically specified reachability, append G_6 :

$$\begin{aligned} \mathcal{G}_{\text{epox}}^{\chi} &= \mathcal{G}_{\text{epox}}^{\text{conn}} \cup \{G_6\}, \\ \mathcal{G}_{\text{hyd}}^{\chi} &= \mathcal{G}_{\text{hyd}}^{\text{conn}} \cup \{G_6\}. \end{aligned} \quad (694)$$

This makes explicit that failure of G_2 , G_3 , or G_4 eliminates the canonical epoxide-mediated factorization without, by itself, eliminating the alternative G'_4 branch.

Let

$$\mathcal{R}(P) \quad (695)$$

be the collection of declared proof or realization routes to a target statement P .

For $r \in \mathcal{R}(P)$, let

$$\text{Supp}_{\text{cert}}(r) \subseteq \mathcal{H} \quad (696)$$

be the hypotheses requiring certification along that route.

Definition 11.2 (Minimal certification front). The *minimal certification front* of P is

$$\text{Front}_{\text{cert}}(P) := \min_{\subseteq} \{\text{Supp}_{\text{cert}}(r) : r \in \mathcal{R}(P)\}. \quad (697)$$

Certification of one complete member of $\text{Front}_{\text{cert}}(P)$ is sufficient to instantiate the corresponding target statement within the declared realization framework.

11.5 Certification of substitution invariance

The revised local-transformation theorem of Section 7 requires more than certification of one reference path.

For the selected reference lifts, determine the positive constraint margin

$$m_{\min} > 0. \quad (698)$$

For every $\Lambda \in \mathcal{L}$, the family-level connectivity theorem requires:

a candidate transported lift for every generator,

$$\Delta_{\mathcal{F}}^{\Lambda} < m_{\min}. \quad (699)$$

When the coordinate-space criterion of Corollary 7.16 is used, the sufficient condition may instead be reported as

$$\varepsilon_{\Lambda} < \varepsilon_0, \quad (700)$$

provided existence of the candidate transported lifts has been established independently.

For stereochemical family invariance one additionally requires

$$\sup_t \left| \tilde{\zeta}_{\chi}(t) - \zeta_{\chi}(t) \right| < \delta_{\chi}. \quad (701)$$

Thus the family-level theorem has its own certifiable interface:

$$\begin{aligned} &\text{chemical concordance} \\ &+ \text{candidate geometric transport} \\ &+ \text{constraint-margin preservation} \\ &+ \text{stereochemical-margin preservation when required.} \end{aligned} \quad (702)$$

11.6 Mechanism-discriminating evidence

Persistent atom identities produce experimental observables capable of distinguishing reaction words that reach the same unlabeled product.

For the canonical carbonyl route, Proposition 8.4 gives

$$o_{\text{carbonyl}} = o_x. \quad (703)$$

An isotope-labeled oxygen donor therefore yields the mechanism-specific prediction

$$^{18}o_x \mapsto ^{18}o_{\text{carbonyl}}, \quad (704)$$

whereas labeling the original tether oxygen o_6 does not label the canonical C_{β} carbonyl.

Likewise, a product certificate must distinguish the target bond

$$\bar{b}(v_5, c_{\alpha}) = 1 \quad (705)$$

from alternative chrysene-locant attachment, and must distinguish



from other ribose or nitrogen acylation products.

For stereochemical realization, the product certificate must establish

$$\chi(c_\alpha) = \chi_\star. \quad (707)$$

If the intended product is described as L-configured, the certificate must additionally contain the complete product structure, CIP assignment, and explicit mapping from the resulting absolute configuration to the applicable L/D convention.

Specific spectroscopic, isotopic, structural, and analytical implementations are given in Appendix G.

11.7 Realization-certified theorem statements

For a theorem

$$\Theta : \left(\bigwedge_{H \in \mathcal{H}_\Theta} H \right) \implies P, \quad (708)$$

define its certificate support by

$$\text{Supp}_{\text{cert}}(\Theta) = \mathcal{H}_\Theta. \quad (709)$$

For example,

$$\text{Supp}_{\text{cert}}(\Theta_{\text{conn}}) = \mathbf{H}_{\text{fam}}^{\text{conn}}, \quad (710)$$

while

$$\text{Supp}_{\text{cert}}(\Theta_\chi) = \mathbf{H}_{\text{fam}}^\chi. \quad (711)$$

Definition 11.3 (Realization-certified theorem). A conditional theorem Θ is *realization certified* for a specified molecular realization $\mathcal{R}$ when

$$\nu(H) = \text{C} \quad \text{for every } H \in \text{Supp}_{\text{cert}}(\Theta). \quad (712)$$

Theorem 11.4 (Certificate lifting of a conditional reachability theorem). *Let*

$$\Theta : \left(\bigwedge_{H \in \mathcal{H}_\Theta} H \right) \implies P \quad (713)$$

be a proved conditional theorem.

Suppose that for a specified molecular realization $\mathcal{R}$, every $H \in \mathcal{H}_\Theta$ has a valid realization certificate.

Then P is realization certified for $\mathcal{R}$ relative to the declared certificate system.

Proof. Validity of every required certificate establishes each hypothesis in the antecedent relative to the declared evidence and acceptance criteria. The proved implication then yields P for the certified realization model. $\square$

11.8 Certification states and falsification propagation

It is useful to distinguish three reporting levels.

Conditional mathematical state.

The implication

$$\mathbf{H}_\Theta \implies P$$

has been proved, but at least one realization hypothesis remains uncertified.

Computationally instantiated state.

Every hypothesis required by the selected theorem route has passed its declared computational certificate within the stated method, resolution, and uncertainty limits.

Experimentally instantiated state.

The defining structural, connectivity, atom-provenance, and stereochemical hypotheses required by the selected theorem route have received the declared experimental certificates.

If

$$\nu(H_j) = \text{F}, \quad (714)$$

then every realization route whose certificate support necessarily contains H_j is eliminated for that molecular realization.

However,

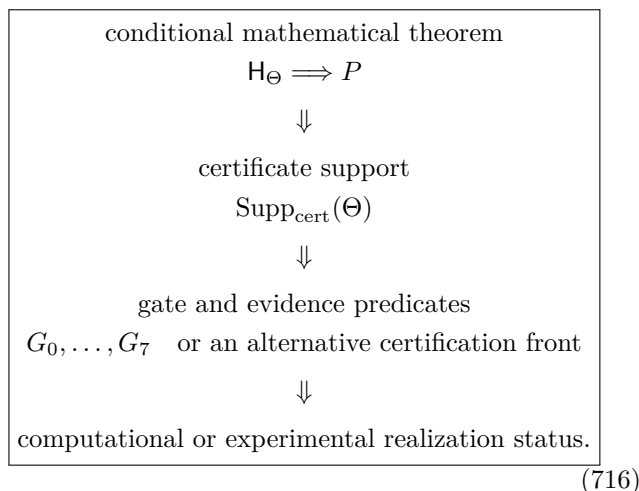
$$\text{falsification of one reaction route} \not\Rightarrow \text{falsification of target reachability} \quad (715)$$

whenever another complete certification front remains available.

For example, failure of the epoxide-mediated carbonyl branch removes the route containing $\{G_2, G_3, G_4\}$, but leaves the G'_4 hydroxylation-oxidation route available for independent certification.

11.9 Certification summary

The certification architecture of the paper may therefore be written:



The main text therefore records the logical certification interface. Appendix G contains the detailed computational hierarchies, uncertainty treatment, ensemble criteria, isotope-labeling strategies, spectroscopic product assignments, competing-pathway analyses, dual-cipher comparisons, adenine-anchor comparisons, and prospective computational and experimental workflows.

12 Discussion and Interpretation

The mathematical construction developed in the preceding sections addresses a constrained existence problem: whether the specified chrysene-adenosine realization can be represented by a typed reaction system in which the reference molecular state admits at least one finite cage-constrained path to the target molecular architecture.

The principal result is the Cage-Constrained Transformation Existence Theorem of Section 9. Under the declared reference and locality hypotheses,

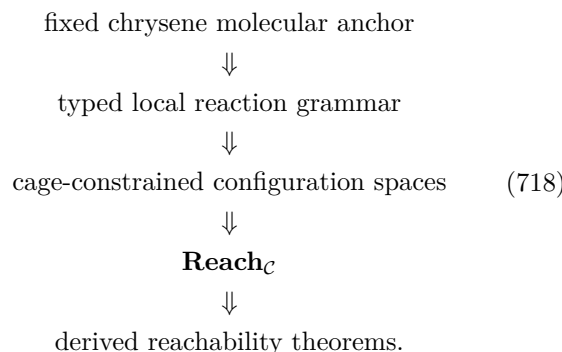
$$\begin{aligned}
 &\forall \Lambda \in \mathcal{L}, \\
 &\exists T_\star^\Lambda \in \mathfrak{T}_\star^\Lambda \text{ such that} \\
 &\text{Hom}_{\text{Reach}_\Lambda^{6 \rightarrow 5}}(S_0^\Lambda, T_\star^\Lambda) \neq \emptyset, \\
 &\chi_{T_\star^\Lambda}(c_\alpha) = \chi_\star.
 \end{aligned}
 \tag{717}$$

The importance of Equation (717) is that connectivity, chemical admissibility, cage accessibility, stereochemical selection, and physical certification are represented as separate mathematical or realization layers rather than being identified by a single reaction drawing.

12.1 From the Chrysene Formalism to a local reaction theory

The present construction is downstream of the Chrysene Formalism. The inherited theory supplies the fixed chrysene molecular anchor, locant data, primary-dual attachment structure, perimeter relations, and directional attachment information.

The reaction theory begins only after those objects have been fixed. Its dependency structure is therefore



This ordering prevents the proposed chemical pathway from becoming a defining property of the underlying chrysene formalism. The molecular framework and the reaction realization remain distinct.

A second central distinction is

chemical graph reachability $\neq$ cage-constrained reachability.

(719)

A chemically admissible rewrite describes an atom-mapped change of molecular state. A cage-constrained transition additionally requires

$$\text{Lift}_C(p; S, S') \neq \emptyset. \tag{720}$$

The cage is therefore represented as a restriction on admissible configuration and path spaces rather than as an informal assertion of molecular proximity.

12.2 Role of the π -stacked adenosine architecture

The adenosine-containing portion of the reference realization performs several logically distinct roles.

First, the adenine aromatic system contributes to the cage geometry through observables such as

$$d_\pi, \quad s_\pi, \quad \Theta_\pi. \tag{721}$$

Second, adenine-, ribose-, linker-, or phosphate-associated atoms may belong to the cage support $C(S)$ without belonging to the chemical reaction support U_{rxn} . They may therefore constrain the geometry of a rewrite while remaining chemically unchanged.

Third, the persistent ribose atom

$$o_{2'} \quad (722)$$

is the terminal acceptor in the target acyl-transfer transformation.

These roles are deliberately separated. Cage organization by the adenosine component does not assign it an automatic redox or catalytic function, and availability of the 2'-oxygen does not itself imply terminal transfer.

The reference realization uses the adenine attachment parameter

$$\eta_A = C2. \quad (723)$$

Its importance in the present theory is principally geometric: changing the anchor may alter

$$d_\pi, s_\pi, \Theta_\pi, d_{\text{cap}}, d_{\text{acyl}}, \quad (724)$$

and the orientation of the stereochemical attack region while leaving the local chemical reaction grammar unchanged.

Thus $C2$ is the reference cage realization rather than an axiomatically unique adenine attachment site.

12.3 Local transformation invariance

A principal result of the paper is that the local chemical reaction word can be separated from remote chrysene substitution.

For the completed support

$$U_{\text{rxn}}, \quad (725)$$

exact local chemical concordance and reaction-inert external context give exact transport of the chemical rewrite word among

$$\mathcal{L} = \{\{6, 12\}, \{3, 6, 12\}, \{3, 6, 9, 12\}\}. \quad (726)$$

The geometric result is necessarily conditional on more information. For a selected reference path, let

$$m_{\min} > 0 \quad (727)$$

be its uniform hard-constraint margin.

For a transported realization Λ , suppose corresponding candidate geometric lifts have been supplied. Their constraint deviation is

$$\Delta_{\mathcal{F}}^\Lambda. \quad (728)$$

The persistence condition

$$\boxed{\Delta_{\mathcal{F}}^\Lambda < m_{\min}} \quad (729)$$

then guarantees that the candidate transports remain cage admissible.

Thus local transformation invariance means:

$$\boxed{\text{the same ordered local rewrite architecture has an admissible transport}} \quad (730)$$

It does not require equality of the complete global conformations. A coordinate-space bound

$$\varepsilon_\Lambda < \varepsilon_0 \quad (731)$$

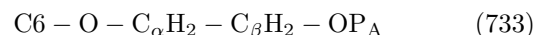
may be used as a sufficient criterion when the continuity assumptions of Corollary 7.16 hold, but existence of the corresponding candidate lifts remains a separate hypothesis.

12.4 The canonical witness and mechanistic resolution

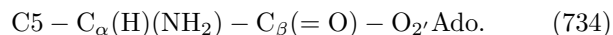
The explicit witness of Section 8 is

$$\Phi_{\text{can}} = p_{\text{tr}} \circ p_{\text{am}} \circ p_{\text{carb}} \circ p_{\text{epox}} \circ p_{\text{unsat}} \circ p_{\text{cap}}. \quad (732)$$

Its net local transformation is



to



The six-generator factorization has a mathematical advantage: it makes atom identity, chemical admissibility, oxygen provenance, stereochemistry, and geometric liftability separately auditable.

It should therefore be interpreted as a chosen resolution of the reaction grammar. A physical realization may justify replacement of several formal generators by one chemically elementary process, or may require a nominal generator to be refined into several additional steps. The reachability framework accommodates either change provided the source and target states, persistent atom maps, and admissibility conditions are updated consistently.

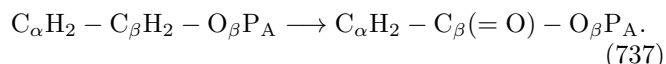
The carbonyl-forming stage illustrates this point directly. The canonical witness uses

$$P_\beta^{\text{epox}} = p_{\text{carb}} \circ p_{\text{epox}} \circ p_{\text{unsat}}, \quad (735)$$

whereas an alternative realization may use

$$P_\beta^{\text{hyd}} = q_{\text{ox}} \circ q_{\text{hyd}}. \quad (736)$$

Both are intended to connect the same local endpoint states:



If both composites are present in the declared cage-constrained grammar, the corresponding reaction words remain distinct morphisms. Target existence therefore need not depend on selecting one unique carbonyl factorization in advance.

12.5 Atom provenance and stereochemical information

Persistent atom identities allow reaction words with the same unlabeled product connectivity to retain experimentally distinguishable information.

For the canonical carbonyl route,

$$o_{\text{carbonyl}} = o_x. \quad (738)$$

The original tether oxygen o_6 does not become the C_β carbonyl oxygen in this witness.

Thus two product-equivalent paths may satisfy

$$\pi_{\text{main}}(T_f) = \pi_{\text{main}}(T_g) \quad (739)$$

while

$$\text{Prov}_f(o_{\text{carbonyl}}) \neq \text{Prov}_g(o_{\text{carbonyl}}). \quad (740)$$

This supplies a direct bridge from the abstract path category to mechanism-discriminating isotope experiments.

The stereochemical result is likewise additional information beyond connectivity.

Connectivity-level existence requires a terminal state in

$$\mathfrak{T}_{\text{conn}}^\Lambda, \quad (741)$$

whereas the stronger target class

$$\mathfrak{T}_\star^\Lambda \subseteq \mathfrak{T}_{\text{conn}}^\Lambda \quad (742)$$

requires

$$\chi(c_\alpha) = \chi_\star. \quad (743)$$

The strong theorem uses geometric branch exclusion:

$$\mathcal{U}_N \cap \mathcal{A}_{\chi_\star} \neq \emptyset, \quad \mathcal{U}_N \cap \mathcal{A}_{\chi_{\text{opp}}} = \emptyset. \quad (744)$$

A realized system may instead exhibit only energetic discrimination

$$\Delta \Delta G_\chi^\ddagger > 0, \quad (745)$$

which supports preferential rather than deterministic selection.

The L-series designation is derived only after the complete product structure has been assigned:

$$\text{oriented cage selection} + \text{CIP assignment} + \text{L/D convention} \implies \chi_\star = \chi_L \quad (746)$$

12.6 Alternative realizations and reaction-word nonuniqueness

The main theorem requires nonemptiness of a target hom-set:

$$\text{Hom}(S_0, T_\star) \neq \emptyset. \quad (747)$$

The free reaction category retains additional information whenever more than one ordered generator word reaches the

same target. Accordingly, the later alternative-realization analysis distinguishes:

$$\begin{aligned} &\text{reaction-word nonuniqueness,} \\ &\text{molecular-realization nonuniqueness,} \\ &\text{terminal-coproduct nonuniqueness.} \end{aligned} \quad (748)$$

These are different statements.

The dual-cipher realization provides a second local architecture:

$$C6 \rightarrow C5 \quad \longleftrightarrow \quad C5 \rightarrow C6. \quad (749)$$

Their local reaction grammars may be related by the support transport

$$\Sigma_{56}, \quad (750)$$

but Σ_{56} is not thereby promoted to a Euclidean symmetry of the chemically instantiated molecule. Reaction barriers, cage geometries, and stereochemical discrimination may therefore differ between the paired realizations.

Adenine-anchor variation gives a second type of realization transport:

$$C2 \longrightarrow N6. \quad (751)$$

If the anchor change lies outside the chemical support, the local rewrite word may transport exactly while its cage realization changes.

These constructions suggest interpreting the target not as the output of one unique microscopic trajectory but through the realization family

$$\mathcal{R}(T_\star) = \{p : S_0^p \preceq_c T_\star^p\}. \quad (752)$$

The first existence question is therefore

$$\mathcal{R}(T_\star) \neq \emptyset. \quad (753)$$

Subsequent physical analysis may then determine which members of this family are experimentally instantiated and which provide the most favorable kinetic or stereochemical behavior.

12.7 Conditional mathematics and physical certification

The mathematical and realization levels are joined by the certificate framework of Section 11.

For a proved theorem

$$\Theta : \mathbf{H}_\Theta \implies P, \quad (754)$$

the physical problem is to determine whether the specified molecular realization satisfies every hypothesis in

$$\text{Supp}_{\text{cert}}(\Theta). \quad (755)$$

This produces the hierarchy

$$\begin{array}{c}
 \text{typed chemical admissibility} \\
 \Downarrow \\
 \text{cage liftability} \\
 \Downarrow \\
 \text{energetic accessibility} \\
 \Downarrow \\
 \text{observable reaction behavior.}
 \end{array} \tag{756}$$

Each successive level uses information not supplied by the preceding one.

The certification-front construction is particularly useful for nonunique reaction systems. For example, failure of the canonical epoxide-mediated carbonyl route eliminates one realization route, while an independently certified hydroxylation-oxidation route may still support the common target statement.

The relevant empirical question is therefore

$$\boxed{\text{Does at least one complete certification front survive?}} \tag{757}$$

This formulation permits competing mechanisms to be tested independently without embedding their physical validity into the mathematical proof itself.

12.8 Extensions and overall interpretation

Several mathematical extensions follow naturally from the present construction.

One direction is to replace the free reaction category by a quotient that identifies independently commuting transformations. Another is to introduce a physically informed path cost

$$A_{\text{phys}}(f) \tag{758}$$

and study variational selection over

$$\text{Hom}(S, T). \tag{759}$$

A stochastic extension could equip reaction paths or cage configurations with probability measures, replacing purely existential reachability by ensemble-weighted reachability. Time-dependent cage domains, thermally weighted configuration measures, or higher-categorical descriptions of coupled chemical and geometric transformations provide further possible developments.

The molecular realization class can likewise be enlarged by varying tether length, phosphate architecture, adenine-side linker structure, stack registry, auxiliary hydrogen-bonding groups, redox components, or coordination sites. Such changes may be represented by new realization parameters p and corresponding categories

$$\text{Reach}_C^p. \tag{760}$$

The conceptual result of the present work can therefore be summarized vertically:

$$\begin{array}{c}
 \text{C6} - \text{O} - \text{C}_\alpha\text{H}_2 - \text{C}_\beta\text{H}_2 - \text{OPO}_3\text{R}_A \\
 \Downarrow \quad \text{typed local chemical transformations} \\
 \text{cage-constrained path space} \\
 \Downarrow \quad \text{geometric and stereochemical selection} \\
 \text{C5} - \text{C}_\alpha(\text{H})(\text{NH}_2) - \text{C}_\beta(=\text{O}) - \text{O}_2'\text{Ado} \\
 \Downarrow \\
 \text{transport across an admissible realization family.}
 \end{array} \tag{761}$$

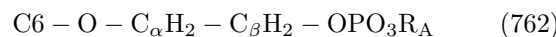
The resulting theory is therefore most naturally interpreted as a constructive existence and local-invariance framework for constrained molecular transformation. The reaction grammar supplies the chemical topology, the cage restricts the admissible geometric paths, persistent atom identities retain mechanistic provenance, and the stereochemical layer selects the target configuration when its stronger hypotheses hold.

Section 13 summarizes these results and the resulting validation program.

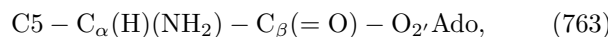
13 Conclusion

This work develops a mathematical existence theory for constrained chemical transformation in a π -stacked chrysene-adenosine architecture. The construction begins with a fixed chrysene molecular anchor and adds a persistent atom universe, a typed local reaction grammar, cage-constrained configuration spaces, and a reaction category whose morphisms are finite compositions of chemically admissible, geometrically liftable transformations.

The reference molecular problem is the transformation of the saturated local tether



to the target architecture



while preserving the inherited C5 – C6 chrysene carbon-framework edge.

The principal mathematical result is the Cage-Constrained Transformation Existence Theorem. Under the reference chemical, structural, cage, terminal-bookkeeping, and stereochemical hypotheses together with

the family-level locality conditions,

$$\boxed{\begin{aligned} &\forall \Lambda \in \mathcal{L}, \\ &\exists T_{\star}^{\Lambda} \in \mathfrak{T}_{\star}^{\Lambda} \text{ such that} \\ &\text{Hom}_{\mathbf{Reach}_{\Lambda}^{6 \rightarrow 5}}(S_0^{\Lambda}, T_{\star}^{\Lambda}) \neq \emptyset, \\ &\chi_{T_{\star}^{\Lambda}}(c_{\alpha}) = \chi_{\star}. \end{aligned}} \quad (764)$$

A weaker theorem establishes the same target connectivity without requiring stereochemical selection. Accordingly, the theory separates

$$\text{connectivity existence} \quad (765)$$

from

$$\text{stereochemically specified existence.} \quad (766)$$

The proof is constructive. One explicit witness is

$$\Phi_{\text{can}} = p_{\text{tr}} \circ p_{\text{am}} \circ p_{\text{carb}} \circ p_{\text{epox}} \circ p_{\text{unsat}} \circ p_{\text{cap}}. \quad (767)$$

This finite word preserves persistent atom identities, maintains the protected chrysene framework, forms the C_5-C_{α} bond, generates the C_{β} carbonyl, installs the amino substituent at C_{α} , and forms the terminal $C_{\beta}-O_{2'}$ bond. For the canonical carbonyl factorization, the atom map further gives the mechanism-specific provenance relation

$$o_{\text{carbonyl}} = o_x. \quad (768)$$

The locality theory separates exact graph transport from geometric persistence. Remote substitution outside the completed chemical reaction support preserves the ordered local rewrite word under exact chemical concordance. For the corresponding cage path, persistence requires supplied candidate geometric transports whose hard-constraint deviation satisfies

$$\Delta_{\mathcal{F}}^{\Lambda} < m_{\min}. \quad (769)$$

Under this condition, the same local reaction architecture remains cage admissible across

$$\mathcal{L} = \{\{6, 12\}, \{3, 6, 12\}, \{3, 6, 9, 12\}\}. \quad (770)$$

When the transported amino-installation path also remains within the stereochemical margin, the selected configuration $\chi_{\star}$ is preserved. Identification of $\chi_{\star}$ with an intended L-series product is made only after the full stereochemical assignment and applicable L/D convention are supplied.

The reaction category intentionally retains distinct reaction words. Consequently, the canonical epoxide-mediated carbonyl route

$$P_{\beta}^{\text{epox}} = p_{\text{carb}} \circ p_{\text{epox}} \circ p_{\text{unsat}} \quad (771)$$

may coexist with alternative factorizations such as

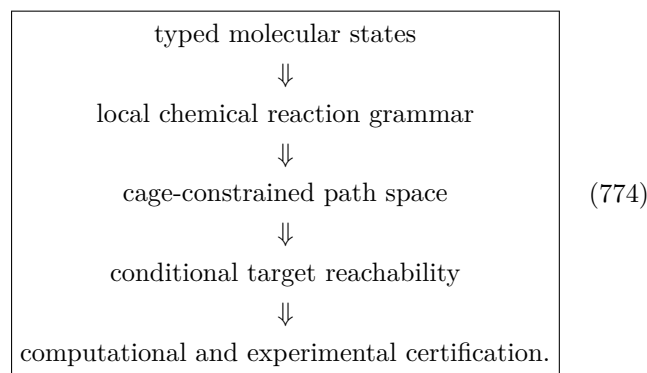
$$P_{\beta}^{\text{hyd}} = q_{\text{ox}} \circ q_{\text{hyd}}. \quad (772)$$

Dual-cipher transport and adenine-anchor variation provide further realization alternatives. These constructions preserve the distinction between existence of a target-reaching path and uniqueness of either the reaction word or the molecular realization.

The physical interpretation of the theorem is organized through the certification framework

$$G_0, \dots, G_7, \quad (773)$$

together with alternative certification fronts when multiple reaction routes are available. Thus the final logical structure is



The principal contribution is therefore a constructive mathematical framework in which chemical connectivity, cage accessibility, stereochemical selection, realization transport, and physical certification can be evaluated as distinct but composable statements. The immediate next step is to determine which members of the formally admissible realization family are supported by computation and experiment and which reaction words are physically instantiated within those realizations.

A Persistent Atom Registry and Local State Concordance

This appendix records the persistent atom identities used in the canonical $C6 \rightarrow C5$ construction and gives an explicit concordance among the local states

$$S_0^\Lambda, \dots, S_6^\Lambda.$$

Its purpose is to make atom conservation, hydrogen transfer, bond provenance, and terminal connectivity independently auditable.

A.1 Closed atom universe and resource bookkeeping

For a fixed realization, let

$$\mathbb{A} = \mathbb{A}_{\text{core}} \sqcup \mathbb{A}_{\text{Ado}} \sqcup \mathbb{A}_{\text{reag}} \sqcup \mathbb{A}_{\text{aux}} \quad (775)$$

be the persistent atom universe, where:

$$\begin{aligned} \mathbb{A}_{\text{core}} &= \text{chrysene and tether atoms,} \\ \mathbb{A}_{\text{Ado}} &= \text{adenine, ribose, linker, and phosphate atoms,} \\ \mathbb{A}_{\text{reag}} &= \text{atoms supplied by explicit chemical reagents,} \\ \mathbb{A}_{\text{aux}} &= \text{explicit counterion or auxiliary atoms.} \end{aligned} \quad (776)$$

Every complete atom-balanced state uses the same atom set:

$$V(S_i) = \mathbb{A} \quad (0 \leq i \leq 6). \quad (777)$$

Connected components and bond relations may change, but persistent atom identity does not.

Abstract resource labels such as e^- , H^+ , or $h\nu$ belong to the resource ledger $\mathcal{R}$ unless the selected realization explicitly represents the corresponding particle or atom as a member of $\mathbb{A}$. Thus resource bookkeeping and atom bookkeeping are not identified.

A.2 Distinguished persistent heavy atoms

The principal heavy atoms are:

v_5	Chrysene carbon at inherited locant $C5$.
v_6	Chrysene carbon at inherited locant $C6$.
o_6	Original oxygen of the $C6 - O - C_\alpha$ tether.
c_α	Proximal tether carbon and eventual stereogenic α -carbon.
c_β	Distal tether carbon and eventual acyl carbon.
o_β	Original oxygen connecting c_β to the phosphate-containing domain.
p	Persistent phosphorus atom of the phosphate-containing domain.
$o_{2'}$	Persistent adenosine ribose 2'-oxygen.

o_x Externally supplied oxygen used as the carbonyl oxygen in the canonical oxygenation/carbonyl factorization.

n_α Externally supplied nitrogen that becomes the amino nitrogen at c_α .

The same symbol denotes the same persistent atom in every state.

A.3 Distinguished persistent hydrogen atoms

Choose the persistent hydrogen identities

$$h_5, \quad h_{\alpha,1}, h_{\alpha,2}, \quad h_{\beta,1}, h_{\beta,2}, \quad h_{2'}. \quad (778)$$

Their initial assignments are:

$$\begin{aligned} h_5 &: v_5 - H, \\ h_{\alpha,1}, h_{\alpha,2} &: c_\alpha - H, \\ h_{\beta,1}, h_{\beta,2} &: c_\beta - H, \\ h_{2'} &: o_{2'} - H. \end{aligned} \quad (779)$$

For the canonical atom map we choose:

$$h_{\alpha,2}, h_{\beta,2} \quad (780)$$

as the hydrogens removed from the principal component during p_{unsat} , and

$$h_{\beta,1} \quad (781)$$

as the hydrogen transferred from c_β to c_α during p_{carb} .

Hydrogens associated with the nitrogen-transfer reagent are likewise persistent atoms in $\mathbb{A}_{\text{reag}}$ when represented explicitly. Their detailed reagent-side identities depend on the selected balanced amination realization and are not fixed by the principal local projection.

A.4 Initial local graph

The initial reactive heavy-atom path is

$$v_6 - o_6 - c_\alpha - c_\beta - o_\beta - p. \quad (782)$$

The initially absent target bonds satisfy

$$\bar{b}_{S_0}(v_5, c_\alpha) = 0, \quad (783)$$

$$\bar{b}_{S_0}(c_\alpha, n_\alpha) = 0, \quad (784)$$

and

$$\bar{b}_{S_0}(c_\beta, o_{2'}) = 0. \quad (785)$$

The inherited chrysene edge is protected:

$$\bar{b}_{S_i}(v_5, v_6) = \bar{b}_{G_{\text{chr}}}(v_5, v_6) \quad (0 \leq i \leq 6). \quad (786)$$

A.5 State-by-state heavy-atom concordance

The principal local motifs are:

$$\begin{aligned}
 S_0^\Lambda &: \text{C6} - \text{O}_6 - \text{C}_\alpha\text{H}_2 - \text{C}_\beta\text{H}_2 - \text{O}_\beta\text{P}_\text{A}, \\
 S_1^\Lambda &: \text{C5} - \text{C}_\alpha\text{H}_2 - \text{C}_\beta\text{H}_2 - \text{O}_\beta\text{P}_\text{A} \quad \text{with } \text{C6} - \text{O}_6\text{H}, \\
 S_2^\Lambda &: \text{C5} - \text{C}_\alpha\text{H} = \text{C}_\beta\text{H} - \text{O}_\beta\text{P}_\text{A}, \\
 S_3^\Lambda &: \text{C5} - [\text{C}_\alpha\text{H} - \text{C}_\beta\text{H}(\text{O}_\beta\text{P}_\text{A})] - \text{O}_{\text{xepoxide}}, \\
 S_4^\Lambda &: \text{C5} - \text{C}_\alpha\text{H}_2 - \text{C}_\beta(=\text{O}_\text{x}) - \text{O}_\beta\text{P}_\text{A}, \\
 S_5^\Lambda &: \text{C5} - \text{C}_\alpha(\text{H})(\text{NH}_2) - \text{C}_\beta(=\text{O}_\text{x}) - \text{O}_\beta\text{P}_\text{A}, \\
 S_6^\Lambda &: \text{C5} - \text{C}_\alpha(\text{H})(\text{NH}_2) - \text{C}_\beta(=\text{O}_\text{x}) - \text{O}_{2'}\text{Ado} + \text{Z}_\text{P}.
 \end{aligned} \tag{787}$$

These expressions display only the principal local molecular component. Every complete state also contains the reagent, counterion, hydrogen, and coproduct components required by the selected balanced realization.

A.6 Hydrogen concordance

The hydrogen identities attached to the principal reactive atoms evolve as follows.

Initially,

$$\begin{aligned}
 H_{S_0}(v_5) &= \{h_5\}, \\
 H_{S_0}(c_\alpha) &= \{h_{\alpha,1}, h_{\alpha,2}\}, \\
 H_{S_0}(c_\beta) &= \{h_{\beta,1}, h_{\beta,2}\}.
 \end{aligned} \tag{788}$$

After capture,

$$H_{S_1}(o_6) \supseteq \{h_5\}, \tag{789}$$

while the c_α and c_β hydrogen sets remain unchanged.

After unsaturation,

$$H_{S_2}(c_\alpha) = \{h_{\alpha,1}\}, \quad H_{S_2}(c_\beta) = \{h_{\beta,1}\}, \tag{790}$$

and

$$h_{\alpha,2}, h_{\beta,2} \tag{791}$$

have entered declared hydrogen-sink or reagent-side states.

Oxygen addition does not change these assignments:

$$H_{S_3}(c_\alpha) = \{h_{\alpha,1}\}, \quad H_{S_3}(c_\beta) = \{h_{\beta,1}\}. \tag{792}$$

The carbonyl-forming rearrangement transfers $h_{\beta,1}$ to c_α :

$$\boxed{H_{S_4}(c_\alpha) = \{h_{\alpha,1}, h_{\beta,1}\}, \quad H_{S_4}(c_\beta) = \emptyset.} \tag{793}$$

Accordingly, the hydrogen replaced during amino installation must satisfy

$$\boxed{h_{\alpha,\text{am}} \in \{h_{\alpha,1}, h_{\beta,1}\}.} \tag{794}$$

Define the retained α -hydrogen by

$$h_{\alpha,\text{rem}} \in \{h_{\alpha,1}, h_{\beta,1}\} \setminus \{h_{\alpha,\text{am}}\}. \tag{795}$$

Then

$$H_{S_5}(c_\alpha) = H_{S_6}(c_\alpha) = \{h_{\alpha,\text{rem}}\}. \tag{796}$$

At terminal acyl transfer, $h_{2'}$ leaves $o_{2'}$ and enters the explicitly modeled phosphate/proton-transfer coproduct domain.

A.7 Persistent atom provenance

Persistent atom identity gives

$$v_5 \mapsto v_5, \quad v_6 \mapsto v_6, \tag{797}$$

$$c_\alpha \mapsto c_\alpha, \quad c_\beta \mapsto c_\beta, \tag{798}$$

and, for the canonical witness,

$$o_x \mapsto o_{\text{carbonyl}}, \quad o_{2'} \mapsto o_{\text{ester}}. \tag{799}$$

Hence

$$\boxed{\text{Prov}_{\Phi_{\text{can}}}(o_{\text{carbonyl}}) = o_x,} \tag{800}$$

and

$$\boxed{\text{Prov}_{\Phi_{\text{can}}}(o_{\text{ester}}) = o_{2'}.} \tag{801}$$

A.8 Principal bond-change concordance

The six canonical generators have the following principal effects:

$$\begin{aligned}
 p_{\text{cap}} : \quad & o_6 - c_\alpha \text{ deleted}, \quad v_5 - c_\alpha \text{ formed}, \\
 & v_5 - h_5 \text{ deleted}, \quad o_6 - h_5 \text{ formed};
 \end{aligned}$$

$$\begin{aligned}
 p_{\text{unsat}} : \quad & c_\alpha - c_\beta \text{ single} \longrightarrow c_\alpha = c_\beta, \\
 & c_\alpha - h_{\alpha,2}, \quad c_\beta - h_{\beta,2} \text{ transferred};
 \end{aligned}$$

$$\begin{aligned}
 p_{\text{epox}} : \quad & c_\alpha = c_\beta \longrightarrow c_\alpha - c_\beta, \\
 & c_\alpha - o_x \text{ and } c_\beta - o_x \text{ formed};
 \end{aligned}$$

$$\begin{aligned}
 p_{\text{carb}} : \quad & c_\alpha - o_x \text{ deleted}, \quad c_\beta - o_x \text{ single} \longrightarrow c_\beta = o_x, \\
 & c_\beta - h_{\beta,1} \text{ deleted}, \quad c_\alpha - h_{\beta,1} \text{ formed};
 \end{aligned}$$

$$p_{\text{am}} : \quad c_\alpha - h_{\alpha,\text{am}} \text{ deleted}, \quad c_\alpha - n_\alpha \text{ formed};$$

$$p_{\text{tr}} : \quad c_\beta - o_\beta \text{ deleted}, \quad c_\beta - o_{2'} \text{ formed}. \tag{802}$$

A bond-order change is represented in the labeled rewrite category by removal of the old labeled edge followed by insertion of the new labeled edge.

A.9 Displayed projection and balanced completion

Let

$$\pi_{\text{disp}} \quad (803)$$

denote projection from a complete atom-balanced state or rule to the displayed local reaction subgraph.

For a displayed local rule p , a *balanced completion* is a complete rule

$$\hat{p} \quad (804)$$

on the fixed atom universe satisfying

$$\pi_{\text{disp}}(\hat{p}) = p. \quad (805)$$

A balanced completion must satisfy the atom-, resource-, and charge-conservation requirements of Section 4.

The local diagrams used in the main text therefore specify the principal transformation exactly while leaving reagent-specific spectator bonds, proton relays, redox partners, and coproduct connectivity to the selected complete realization.

B Explicit Local Rewrite Rules

This appendix records the canonical generators in vertex-preserving labeled graph-rewrite form.

The principal local rules are exact at the displayed atom-map level. When reagent-side structures are not fixed by the abstract model, their complete atom-balanced realization is represented by a balanced completion $\hat{p}$ as defined in Appendix A.9.

B.1 Vertex-preserving rewrite convention

For a local rule p , write

$$p = \left(L_p \xleftarrow{\ell_p} K_p \xrightarrow{r_p} R_p, \Delta q_p, \Delta r_p, \Delta \chi_p, \Delta \rho_p \right). \quad (806)$$

The maps ℓ_p and r_p are injective and preserve persistent atom identity and element type.

For the principal canonical grammar, vertices are not created or destroyed. Chemical change is represented by changes in labeled edges and state labels.

Define

$$E_p^- := E(L_p) \setminus E(K_p) \quad (807)$$

and

$$E_p^+ := E(R_p) \setminus E(K_p). \quad (808)$$

Bond-order replacement is represented by placing the old labeled edge in E_p^- and the new labeled edge in E_p^+ .

Recall

$$\text{Pat}(p) = V(L_p) \cup V(R_p) \quad (809)$$

and

$$\text{Act}(p) \subseteq \text{Pat}(p), \quad (810)$$

where $\text{Act}(p)$ contains every atom incident to a changed bond or carrying a changed charge, radical, or stereochemical label.

Atoms required only as unchanged matching context lie in $\text{Pat}(p) \setminus \text{Act}(p)$.

B.2 Capture rule

The principal displayed pattern contains

$$\{v_5, v_6, o_6, c_\alpha, h_5\}. \quad (811)$$

The deletion set is

$$E_{\text{cap}}^- = \{\{o_6, c_\alpha\}_1, \{v_5, h_5\}_1\}, \quad (812)$$

and the insertion set is

$$E_{\text{cap}}^+ = \{\{v_5, c_\alpha\}_1, \{o_6, h_5\}_1\}. \quad (813)$$

The inherited edge

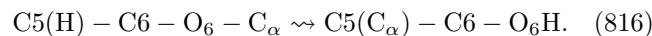
$$\{v_5, v_6\} \quad (814)$$

and the $v_6 - o_6$ bond belong to the preserved interface.

The active set is therefore

$$\text{Act}(p_{\text{cap}}) = \{v_5, o_6, c_\alpha, h_5\}. \quad (815)$$

At the displayed level,



Any realization-specific charge, radical, excitation, or reagent changes are supplied by $\hat{p}_{\text{cap}}$ and must satisfy global charge and resource balance.

B.3 Unsaturation rule

The canonical atom map selects

$$h_{\alpha,2}, \quad h_{\beta,2} \quad (817)$$

for transfer out of the principal component.

The principal deletion set is

$$E_{\text{unsat}}^- = \{\{c_\alpha, c_\beta\}_1, \{c_\alpha, h_{\alpha,2}\}_1, \{c_\beta, h_{\beta,2}\}_1\}, \quad (818)$$

while

$$E_{\text{unsat}}^+ = \{\{c_\alpha, c_\beta\}_2\} \cup E_{\mathcal{Z}_H}^+. \quad (819)$$

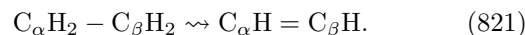
Here $E_{\mathcal{Z}_H}^+$ contains the realization-specific bonds by which $h_{\alpha,2}$ and $h_{\beta,2}$ enter explicitly represented hydrogen-accepting or coproduct states.

The displayed active set contains

$$\{c_\alpha, c_\beta, h_{\alpha,2}, h_{\beta,2}\}, \quad (820)$$

together with any reagent atoms whose bonds are changed in the selected balanced completion.

The local projected rule is



B.4 Oxygen-addition rule

The principal reactive atoms are

$$\{c_\alpha, c_\beta, o_x\}, \quad (822)$$

together with the donor-side atoms needed by the chosen balanced completion.

The principal deletion set is

$$E_{\text{epox}}^- = \{\{c_\alpha, c_\beta\}_2\} \cup E_{\text{donor}}^-, \quad (823)$$

and

$$E_{\text{epox}}^+ = \{\{c_\alpha, c_\beta\}_1, \{c_\alpha, o_x\}_1, \{c_\beta, o_x\}_1\} \cup E_{\text{donor}}^+. \quad (824)$$

The sets $E_{\text{donor}}^\pm$ encode the explicitly selected oxygen-donor fate.

The projected rule is

$$C_\alpha = C_\beta \rightsquigarrow [C_\alpha - C_\beta - O_x]_{\text{epoxide}}. \quad (825)$$

B.5 Carbonyl-forming rearrangement rule

The canonical atom map takes

$$h_{\beta,1} \quad (826)$$

to be the hydrogen transferred from c_β to c_α .

The deletion set is

$$E_{\text{carb}}^- = \{\{c_\alpha, o_x\}_1, \{c_\beta, o_x\}_1, \{c_\beta, h_{\beta,1}\}_1\}, \quad (827)$$

and the insertion set is

$$E_{\text{carb}}^+ = \{\{c_\beta, o_x\}_2, \{c_\alpha, h_{\beta,1}\}_1\}. \quad (828)$$

The bonds

$$\{c_\alpha, c_\beta\}_1 \quad (829)$$

and

$$\boxed{\{c_\beta, o_\beta\}_1} \quad (830)$$

belong to the preserved interface.

Thus

$$[C_\alpha H - C_\beta H(O_\beta P_A)] - O_{x_{\text{epoxide}}} \quad (831)$$

is mapped to

$$C_\alpha H_2 - C_\beta (= O_x) - O_\beta P_A. \quad (832)$$

The defining atom-provenance relation is

$$o_{\text{carbonyl}} = o_x. \quad (833)$$

B.6 Amino-installation rule

Immediately before amino installation, Appendix A.6 gives

$$H_{S_4}(c_\alpha) = \{h_{\alpha,1}, h_{\beta,1}\}. \quad (834)$$

Therefore select

$$\boxed{h_{\alpha,\text{am}} \in \{h_{\alpha,1}, h_{\beta,1}\}}. \quad (835)$$

The hydrogen $h_{\alpha,2}$ is not an admissible choice because it left the principal component during p_{unsat} .

Let E_N^- and E_N^+ encode the selected balanced nitrogen-donor transformation.

Then

$$E_{\text{am}}^- = \{\{c_\alpha, h_{\alpha,\text{am}}\}_1\} \cup E_N^-, \quad (836)$$

and

$$E_{\text{am}}^+ = \{\{c_\alpha, n_\alpha\}_1\} \cup E_N^+. \quad (837)$$

The balanced completion must account explicitly for the hydrogen atoms of the final NH_2 group and for the fate of $h_{\alpha,\text{am}}$.

The projected connectivity change is

$$C_\alpha H_2 \rightsquigarrow C_\alpha(H)(NH_2). \quad (838)$$

The edge rewrite alone does not determine an absolute configuration. For the stereochemically refined generator, the cage-selected branch supplies

$$\Delta\chi_V(c_\alpha) : \perp \mapsto \chi_\star. \quad (839)$$

Thus the stereochemical label is conditioned on the oriented cage-lift realization rather than inferred from an unlabeled graph rewrite.

B.7 Terminal acyl-transfer rule

Let a_P denote the proton acceptor selected within the departing phosphate-containing realization.

The principal deletion set is

$$E_{\text{tr}}^- = \{\{c_\beta, o_\beta\}_1, \{o_{2'}, h_{2'}\}_1\}, \quad (840)$$

and a direct proton-transfer completion may use

$$E_{\text{tr}}^+ = \{\{c_\beta, o_{2'}\}_1, \{a_P, h_{2'}\}_1\}. \quad (841)$$

A realization containing a multi-step proton relay may replace the single $a_P - h_{2'}$ insertion by a finite balanced proton-transfer subpath.

The carbonyl edge

$$\{c_\beta, o_x\}_2 \quad (842)$$

belongs to the preserved interface.

The principal projected rule is

$$C_\beta (= O_x) - O_\beta P_A + HO_{2'} \text{Ado} \rightsquigarrow C_\beta (= O_x) - O_{2'} \text{Ado} + Z_P. \quad (843)$$

B.8 Canonical pattern support

Let

$$\mathcal{P}_{\text{can}} = \{p_{\text{cap}}, p_{\text{unsat}}, p_{\text{epox}}, p_{\text{carb}}, p_{\text{am}}, p_{\text{tr}}\}. \quad (844)$$

The completed chemical support is

$$U_{\text{rxn}} = U_6 \cup \bigcup_{p \in \mathcal{P}_{\text{can}}} \text{Pat}(p). \quad (845)$$

This set contains the displayed reactive atoms together with every reagent-side or unchanged matching atom that is actually inspected by a selected rule.

Under the remote-context hypothesis of Section 7, the additional *C3*, *C9*, and remote *C12* decorations lie outside this completed pattern support.

B.9 Canonical composition and net bond delta

The canonical word is

$$\Phi_{\text{can}} = p_{\text{tr}} \circ p_{\text{am}} \circ p_{\text{carb}} \circ p_{\text{epox}} \circ p_{\text{unsat}} \circ p_{\text{cap}}. \quad (846)$$

At the complete balanced-state level,

$$t(p_i) = s(p_{i+1}) \quad (847)$$

for every consecutive pair.

After cancellation of intermediate bonds, the principal persistent net changes include

$$\bar{b}(v_5, c_\alpha) : 0 \mapsto 1, \quad (848)$$

$$\bar{b}(o_6, c_\alpha) : 1 \mapsto 0, \quad (849)$$

$$\bar{b}(c_\alpha, n_\alpha) : 0 \mapsto 1, \quad (850)$$

$$\bar{b}(c_\beta, o_x) : 0 \mapsto 2, \quad (851)$$

$$\bar{b}(c_\beta, o_\beta) : 1 \mapsto 0, \quad (852)$$

and

$$\bar{b}(c_\beta, o_{2'}) : 0 \mapsto 1. \quad (853)$$

The inherited chrysene carbon-skeleton graph remains unchanged.

C Explicit Cage Constraints and Stereochemical Geometry

This appendix collects the state and transition constraints used by the cage-liftability theory.

A central distinction is made between:

$$\text{closed inequality constraints} \quad (854)$$

and

$$\text{exact equality constraints.} \quad (855)$$

The positive-margin perturbation arguments apply to the former. Exact equalities must either transport exactly or be replaced prospectively by finite tolerance intervals.

C.1 State constraints

For a state S , let

$$C(S) \quad (856)$$

be its finite cage support and let

$$\text{Conf}(C(S)) \quad (857)$$

be the corresponding reduced configuration space.

Let

$$F_{S,j} : \text{Conf}(C(S)) \longrightarrow \mathbb{R}, \quad j \in J_S, \quad (858)$$

be a finite family of continuous inequality functionals.

Let

$$H_{S,k} : \text{Conf}(C(S)) \longrightarrow \mathbb{R}, \quad k \in K_S, \quad (859)$$

be a finite family of exact equality constraints.

Then

$$\mathcal{K}_C(S) = \{x : F_{S,j}(x) \leq 0 \ \forall j, \quad H_{S,k}(x) = 0 \ \forall k\}. \quad (860)$$

The full-state cage set is the inverse image of $\mathcal{K}_C(S)$ under the cage-support projection defined in Section 5.

C.2 Transition constraints

For a chemical rule

$$p : S \longrightarrow S', \quad (861)$$

let

$$\mathcal{X}_p \quad (862)$$

be its transition configuration space.

Let

$$F_{p,j}^{\text{tr}} : \mathcal{X}_p \longrightarrow \mathbb{R} \quad (j \in J_p) \quad (863)$$

be the finite hard inequality family, and let

$$H_{p,k}^{\text{tr}} : \mathcal{X}_p \longrightarrow \mathbb{R} \quad (k \in K_p) \quad (864)$$

be its exact equality family.

The transition-admissible domain is

$$\mathcal{C}_p = \{x \in \mathcal{X}_p : F_{p,j}^{\text{tr}}(x) \leq 0, \quad H_{p,k}^{\text{tr}}(x) = 0\}. \quad (865)$$

A geometric lift must additionally have endpoints in $\mathcal{K}_C(S)$ and $\mathcal{K}_C(S')$.

C.3 Interval constraints

For a continuous observable

$$Y(x) \quad (866)$$

and a closed interval

$$I_Y = [Y_{\min}, Y_{\max}], \quad (867)$$

the condition

$$Y(x) \in I_Y \quad (868)$$

is represented by

$$F_Y^-(x) = Y_{\min} - Y(x) \leq 0 \quad (869)$$

and

$$F_Y^+(x) = Y(x) - Y_{\max} \leq 0. \quad (870)$$

This convention converts every bounded geometric window used below into the common inequality form

$$F(x) \leq 0. \quad (871)$$

C.4 π -stack constraints

The reference stack constraints are

$$d_{\pi}^{\min} \leq d_{\pi}(x) \leq d_{\pi}^{\max}, \quad (872)$$

$$s_{\pi}^{\min} \leq s_{\pi}(x) \leq s_{\pi}^{\max}, \quad (873)$$

and

$$\theta_{\pi}^{\min} \leq \theta_{\pi}(x) \leq \theta_{\pi}^{\max}. \quad (874)$$

The parameter vector

$$\mathbf{c}_{\pi} = (d_{\pi}^{\min}, d_{\pi}^{\max}, s_{\pi}^{\min}, s_{\pi}^{\max}, \theta_{\pi}^{\min}, \theta_{\pi}^{\max}) \quad (875)$$

is realization specific.

C.5 Excluded-volume constraints

For every protected noncoincident atom pair (u, v) , impose

$$d_{uv}(x) \geq r_{\text{ex}}(\epsilon(u), \epsilon(v)) > 0. \quad (876)$$

Equivalently,

$$F_{uv}^{\text{ex}}(x) = r_{\text{ex}}(\epsilon(u), \epsilon(v)) - d_{uv}(x) \leq 0. \quad (877)$$

Positive lower-distance bounds also ensure that the injective configuration domain is closed under the compactness hypotheses used in Appendix D.1.

C.6 Tether-span and orientation constraints

For a declared tether path

$$\mathcal{T} = (a_0, \dots, a_m), \quad (878)$$

define

$$L_{\mathcal{T}}(x) = d_{a_0 a_m}(x). \quad (879)$$

Impose

$$L_{\mathcal{T}}^{\min} \leq L_{\mathcal{T}}(x) \leq L_{\mathcal{T}}^{\max}. \quad (880)$$

When the local orientation scalar π_{ℓ} of Section 2.4 is used, impose

$$\pi_{\ell}^{\min} \leq \pi_{\ell}(x) \leq \pi_{\ell}^{\max}. \quad (881)$$

C.7 Capture constraints

The $C5 - C_{\alpha}$ capture domain is specified by

$$d_{\text{cap}}^{\min} \leq d_{v_5 c_{\alpha}}(x) \leq d_{\text{cap}}^{\max} \quad (882)$$

and

$$\theta_{\text{cap}}^{\min} \leq \theta_{\text{cap}}(x) \leq \theta_{\text{cap}}^{\max}. \quad (883)$$

When a realization requires an additional torsional condition, introduce

$$\phi_{\text{cap}}(x) \quad (884)$$

and impose

$$\phi_{\text{cap}}^{\min} \leq \phi_{\text{cap}}(x) \leq \phi_{\text{cap}}^{\max}. \quad (885)$$

The optional dihedral is not required by the abstract existence framework.

C.8 Oxygen-transfer constraints

For a declared reactive oxygen-donor atom or site z , one may impose

$$d_{z\beta}^{\min} \leq d_{z c_{\beta}}(x) \leq d_{z\beta}^{\max} \quad (886)$$

and a corresponding orientation condition

$$\theta_{z\beta}^{\min} \leq \theta_{z, \alpha, \beta}(x) \leq \theta_{z\beta}^{\max}. \quad (887)$$

For oxygen transfer to the $C_{\alpha} = C_{\beta}$ unit as a whole, these observables may instead be defined relative to the alkene midpoint and local normal.

The specific observable family is part of the realization data.

C.9 Stereochemical attack constraints

Using the oriented frame

$$\mathcal{F}_{\alpha} = (e_1, e_2, e_3) \quad (888)$$

of Section 5.8, define

$$\zeta_{\chi} = \langle u_{\text{att}}, e_3 \rangle. \quad (889)$$

For positive-side attack with robustness margin $\delta_{\chi} > 0$, impose

$$\zeta_{\chi} \geq \delta_{\chi}. \quad (890)$$

For negative-side attack, impose

$$\zeta_{\chi} \leq -\delta_{\chi}. \quad (891)$$

The realization-specific map

$$\kappa_{\alpha} : \{-1, +1\} \longrightarrow \{R, S\} \quad (892)$$

converts the geometric branch into the final absolute configuration after complete substituent ordering.

C.10 Terminal acyl-transfer constraints

Let o_x be the canonical carbonyl oxygen.

Require

$$d_{\text{acyl}}^{\min} \leq d_{c_{\beta}o_{2'}}(x) \leq d_{\text{acyl}}^{\max}, \quad (893)$$

and

$$\theta_{\text{acyl}}^{\min} \leq \theta_{o_x, c_{\beta}, o_{2'}}(x) \leq \theta_{\text{acyl}}^{\max}. \quad (894)$$

A selected realization may append proton-relay or leaving-group orientation constraints without changing the abstract definition of cage liftability.

C.11 Augmented lift constraints including endpoints

For a rule

$$p : S \longrightarrow S', \quad (895)$$

a geometric lift must satisfy both transition constraints and endpoint state constraints.

It is therefore convenient to define the augmented inequality family for a candidate path

$$\gamma : [0, 1] \longrightarrow \mathcal{X}_p. \quad (896)$$

For every transition inequality, define

$$\widehat{F}_{p,j}^{\text{tr}}(\gamma) := \max_{t \in [0,1]} F_{p,j}^{\text{tr}}(\gamma(t)). \quad (897)$$

For reactant-state inequalities, define

$$\widehat{F}_{S,j}^{-}(\gamma) := F_{S,j}(\gamma(0)), \quad (898)$$

and for product-state inequalities,

$$\widehat{F}_{S',j}^{+}(\gamma) := F_{S',j}(\gamma(1)). \quad (899)$$

Collect these finitely many scalar functionals into

$$\widehat{\mathcal{F}}_p. \quad (900)$$

Then the inequality portion of geometric liftability is equivalent to

$$\widehat{F}(\gamma) \leq 0 \quad \text{for every } \widehat{F} \in \widehat{\mathcal{F}}_p. \quad (901)$$

Exact equality constraints are imposed separately:

$$H_{p,k}^{\text{tr}}(\gamma(t)) = 0 \quad (0 \leq t \leq 1), \quad (902)$$

together with

$$H_{S,k}(\gamma(0)) = 0, \quad H_{S',k}(\gamma(1)) = 0. \quad (903)$$

Thus a positive robustness margin is never incorrectly assigned to an exact equality.

C.12 Reference margins and transported deviations

For a reference lift γ and an augmented hard inequality $\widehat{F}_a$, define

$$m_a(\gamma) := -\widehat{F}_a(\gamma). \quad (904)$$

For a finite reference path

$$\Gamma = (\gamma_1, \dots, \gamma_n), \quad (905)$$

define

$$\boxed{m_{\min} := \min_{i,a} m_a(\gamma_i)}. \quad (906)$$

Strict robustness means

$$m_{\min} > 0. \quad (907)$$

For a corresponding candidate transported path $\tilde{\gamma}_i^{\Lambda}$, define transition-function deviation by

$$\Delta_{ij}^{\Lambda, \text{tr}} := \sup_{t \in [0,1]} \left| F_{ij}^{\Lambda, \text{tr}}(\tilde{\gamma}_i^{\Lambda}(t)) - F_{ij}^{\Lambda_0, \text{tr}}(\gamma_i(t)) \right|. \quad (908)$$

Define the corresponding endpoint deviations by

$$\Delta_{ij}^{\Lambda, -} := \left| F_{S_{i-1},j}^{\Lambda}(\tilde{\gamma}_i^{\Lambda}(0)) - F_{S_{i-1},j}^{\Lambda_0}(\gamma_i(0)) \right|, \quad (909)$$

and

$$\Delta_{ij}^{\Lambda, +} := \left| F_{S_i,j}^{\Lambda}(\tilde{\gamma}_i^{\Lambda}(1)) - F_{S_i,j}^{\Lambda_0}(\gamma_i(1)) \right|. \quad (910)$$

Let

$$\boxed{\Delta_{\mathcal{F}}^{\Lambda}} \quad (911)$$

be the maximum over every transition and endpoint deviation entering the finite canonical path.

The perturbative persistence theorem uses

$$\Delta_{\mathcal{F}}^{\Lambda} < m_{\min}, \quad (912)$$

together with exact preservation of the declared equality constraints.

C.13 Soft cage functionals

A realization may additionally define a continuous soft functional

$$\mathcal{E}_{\text{cage}}(x) = E_{\pi}(x) + E_{\text{tether}}(x) + E_{\text{HB}}(x) + E_{\text{el}}(x) + E_{\text{strain}}(x). \quad (913)$$

One may then define the filtered domain

$$\mathcal{K}_C^{E_{\max}}(S) = \{x \in \mathcal{K}_C(S) : \mathcal{E}_{\text{cage}}(x) \leq E_{\max}\}. \quad (914)$$

No theorem in the present paper requires $\mathcal{E}_{\text{cage}}$ to equal an exact molecular free-energy functional.

D Technical Lemmas and Proof Supplements

This appendix collects technical results used in compressed form in the main text.

In particular, it supplies: the corrected compactness argument for the projected cage domain, the exact local context-extension lemma, the quantitative perturbation estimate underlying Section 7, stereochemical sign persistence, the free-category transport property, and the conditional model-theoretic formulation of non-vacuity.

D.1 Compactness of the projected cage domain

The compactness argument is made on the finite cage support rather than on the complete molecular configuration space.

Let

$$C = C(S) \quad (915)$$

be finite and choose one reference atom

$$a_0 \in C. \quad (916)$$

Remove translation by defining the anchored coordinate space

$$\mathcal{X}_0(C) := \{x : C \rightarrow \mathbb{R}^3 : x(a_0) = 0\}. \quad (917)$$

This is naturally identified with

$$\mathbb{R}^{3(|C|-1)}. \quad (918)$$

Lemma D.1 (Compact anchored cage domain). *Assume that the gauge-fixed cage domain*

$$\tilde{\mathcal{K}}_C(S) \subseteq \mathcal{X}_0(C) \quad (919)$$

satisfies:

1. *there exists $R < \infty$ such that*

$$\|x(a)\|_2 \leq R \quad (a \in C) \quad (920)$$

for every $x \in \tilde{\mathcal{K}}_C(S)$;

2. *for every distinct atom pair that must remain noncoincident, there exists $\delta_{ab} > 0$ such that*

$$\|x(a) - x(b)\|_2 \geq \delta_{ab}; \quad (921)$$

3. *every inequality functional defining the domain is continuous; and*
4. *every equality functional defining the domain is continuous.*

Then

$$\tilde{\mathcal{K}}_C(S) \quad (922)$$

is compact.

Proof. The finite-dimensional anchored coordinate space is Euclidean.

Condition (920) gives boundedness.

Every condition

$$F_j(x) \leq 0$$

is closed because F_j is continuous. Every condition

$$H_k(x) = 0$$

is likewise closed.

The positive lower-distance conditions

$$d_{ab}(x) \geq \delta_{ab} > 0$$

are closed and exclude collision limits that would otherwise leave the injective configuration space.

Hence $\tilde{\mathcal{K}}_C(S)$ is a closed bounded subset of a finite-dimensional Euclidean space and is compact by Heine–Borel. $\square$

Corollary D.2 (Compactness modulo proper rotations). *The corresponding projected configuration set modulo $SO(3)$ is compact.*

Proof. The quotient map

$$\tilde{\mathcal{K}}_C(S) \longrightarrow \tilde{\mathcal{K}}_C(S)/SO(3) \quad (923)$$

is continuous. A continuous image of a compact space is compact. $\square$

Corollary D.3 (Minimum of a continuous soft cage functional). *If $\tilde{\mathcal{K}}_C(S) \neq \emptyset$ and*

$$\mathcal{E}_{\text{cage}} : \tilde{\mathcal{K}}_C(S) \longrightarrow \mathbb{R} \quad (924)$$

is continuous, then there exists $x_{\min}$ such that

$$\mathcal{E}_{\text{cage}}(x_{\min}) = \min_{x \in \tilde{\mathcal{K}}_C(S)} \mathcal{E}_{\text{cage}}(x). \quad (925)$$

Proof. Apply the extreme-value theorem. $\square$

D.2 Exact local context extension

Lemma D.4 (Local gluing of a vertex-preserving rewrite). *Let a molecular graph be decomposed as*

$$G = G_U \cup G_X, \quad (926)$$

where U contains the complete pattern footprint of a local rule p and X is external context.

Assume:

1. *p does not alter any external vertex, edge, or label in G_X ;*

2. every edge joining the local pattern to the external context is preserved through the rule interface; and
3. every rule-relevant resource and global state condition has the same admissible value in the compared context.

If

$$p : G_U \rightsquigarrow H_U \quad (927)$$

is a valid local rewrite, then

$$H = H_U \cup G_X \quad (928)$$

is the unique extension relative to the fixed external context.

Proof. The rule changes only data internal to its complete pattern footprint. All local-external incidences appearing in the interface are preserved.

Therefore the same gluing data joining G_U to G_X also join H_U to G_X .

Because the external graph, its labels, and the preserved boundary incidences are fixed, no second context extension exists relative to that external state. $\square$

Proposition D.5 (Finite extension of a local reaction word). *Let*

$$p_n \circ \cdots \circ p_1 \quad (929)$$

be a finite composable reaction word whose complete pattern footprint lies in the same declared local domain U .

If the external context is reaction inert relative to every generator, then the complete word extends uniquely relative to the fixed external context.

Proof. Apply Lemma D.4 to p_1 . The resulting product retains the same external context. Repeat successively for $p_2, \dots, p_n$. Finite induction gives the result. $\square$

D.3 Quantitative persistence of candidate transported lifts

Let the reference path consist of finitely many geometric lifts

$$\gamma_i : [0, 1] \longrightarrow \mathcal{X}_{p_i}^{\Lambda_0}, \quad 1 \leq i \leq n. \quad (930)$$

Let

$$m_{\min} > 0 \quad (931)$$

be the uniform positive margin defined from the complete augmented inequality family of Appendix C.12.

Theorem D.6 (Constraint-deviation persistence). *For a target realization Λ , suppose that for every reference*

generator there is a candidate transported path

$$\tilde{\gamma}_i^\Lambda : [0, 1] \longrightarrow \mathcal{X}_{p_i}^\Lambda \quad (932)$$

having the required transported endpoints and satisfying every exact equality constraint.

If

$$\boxed{\Delta_{\mathcal{F}}^\Lambda < m_{\min}}, \quad (933)$$

then every $\tilde{\gamma}_i^\Lambda$ satisfies all corresponding hard inequality constraints and is therefore a genuine geometric lift.

Proof. For every reference transition inequality,

$$F_{ij}^{\Lambda_0}(\gamma_i(t)) \leq -m_{ij} \leq -m_{\min}. \quad (934)$$

By definition of $\Delta_{\mathcal{F}}^\Lambda$,

$$F_{ij}^\Lambda(\tilde{\gamma}_i^\Lambda(t)) \leq F_{ij}^{\Lambda_0}(\gamma_i(t)) + \Delta_{\mathcal{F}}^\Lambda. \quad (935)$$

Therefore

$$F_{ij}^\Lambda(\tilde{\gamma}_i^\Lambda(t)) \leq -m_{\min} + \Delta_{\mathcal{F}}^\Lambda < 0. \quad (936)$$

The identical estimate applies to the augmented reactant- and product-endpoint inequalities.

All exact equalities hold by hypothesis. Consequently the candidate path lies in the complete transition domain and has endpoints in the corresponding state cage domains. It is therefore a geometric lift. $\square$

Remark D.7 (What the theorem transports). Theorem D.6 is an admissibility-persistence theorem. It does not construct $\tilde{\gamma}_i^\Lambda$; candidate geometric transport is a separate hypothesis.

D.4 Coordinate-space sufficient condition

Let

$$\varphi : C^{\Lambda_0} \longrightarrow C^\Lambda \quad (937)$$

be the persistent cage-support correspondence.

For embedded cage configurations x and $\tilde{x}$, define

$$d_{SE(3), \varphi}(x, \tilde{x}) := \inf_{g \in SE(3)} \max_{a \in C^{\Lambda_0}} \|g x(a) - \tilde{x}(\varphi(a))\|_2. \quad (938)$$

Hypothesis D.8 (Cross-realization modulus of constraint continuity). There exists a function

$$\omega : [0, \infty) \longrightarrow [0, \infty) \quad (939)$$

with

$$\lim_{\varepsilon \rightarrow 0} \omega(\varepsilon) = 0 \quad (940)$$

such that, for corresponding admissible ambient configurations,

$$d_{SE(3),\varphi}(x, \tilde{x}) < \varepsilon \quad (941)$$

implies

$$\left| F_{ij}^{\Lambda}(\tilde{x}) - F_{ij}^{\Lambda_0}(x) \right| \leq \omega(\varepsilon) \quad (942)$$

for every designated hard inequality functional.

This hypothesis compares constraints across different realization spaces. It is stronger than continuity of each F_{ij}^{Λ} separately and is therefore stated explicitly.

Corollary D.9 (Coordinate-space persistence radius). Assume Hypothesis D.8 and $m_{\min} > 0$.

Then there exists

$$\varepsilon_0 > 0 \quad (943)$$

such that

$$\sup_{i,t} d_{SE(3),\varphi}(\gamma_i(t), \tilde{\gamma}_i^{\Lambda}(t)) < \varepsilon_0 \quad (944)$$

implies

$$\Delta_{\mathcal{F}}^{\Lambda} < m_{\min}, \quad (945)$$

provided the required endpoint and equality conditions are satisfied.

Proof. Choose $\varepsilon_0 > 0$ such that

$$\omega(\varepsilon_0) < m_{\min}. \quad (946)$$

The uniform coordinate bound and Hypothesis D.8 then give

$$\Delta_{\mathcal{F}}^{\Lambda} \leq \omega(\varepsilon_0) < m_{\min}. \quad (947)$$

Apply Theorem D.6. $\square$

D.5 Persistence of stereochemical sign

Lemma D.10 (Persistence of the oriented attack branch). Suppose a reference amino-installation trajectory satisfies

$$|\zeta_{\chi}(t)| \geq \delta_{\chi} > 0 \quad (948)$$

throughout the stereochemistry-determining interval. Suppose a transported candidate trajectory satisfies

$$\sup_t \left| \tilde{\zeta}_{\chi}(t) - \zeta_{\chi}(t) \right| < \delta_{\chi}. \quad (949)$$

Then

$$\text{sgn } \tilde{\zeta}_{\chi}(t) = \text{sgn } \zeta_{\chi}(t) \quad (950)$$

throughout that interval.

Proof. For every t ,

$$|\zeta_{\chi}(t)| \geq \delta_{\chi}. \quad (951)$$

If the sign changed under transport, continuity would require the transported scalar to cross zero. At such a point,

$$\left| \tilde{\zeta}_{\chi}(t) - \zeta_{\chi}(t) \right| \geq |\zeta_{\chi}(t)| \geq \delta_{\chi}, \quad (952)$$

contradicting Equation (949). $\square$

This lemma preserves the selected transported stereochemical branch. Global exclusion of every opposite-branch trajectory in the complete perturbed realization is the stronger condition of Definition 5.6.

D.6 Functorial extension of generator transport

Proposition D.11 (Generator transport determines path transport). Let

$$\phi : \mathbb{Q} \longrightarrow \tilde{\mathbb{Q}} \quad (953)$$

be a quiver map preserving source and target. Then there exists a unique functor

$$\text{Free}(\mathbb{Q}) \longrightarrow \text{Free}(\tilde{\mathbb{Q}}) \quad (954)$$

whose action on generating edges is ϕ .

Proof. For a finite path

$$e_n \cdots e_1, \quad (955)$$

define

$$\Phi(e_n \cdots e_1) = \phi(e_n) \cdots \phi(e_1). \quad (956)$$

Source-target preservation guarantees composability.

The empty path is sent to the empty path and concatenation is preserved.

Uniqueness follows because every morphism of a free category is a finite word in its generating edges. $\square$

D.7 Local determination of the principal target

Lemma D.12 (Target-locality). *Suppose two complete terminal states T and $\tilde{T}$ agree on the persistent atom-labeled local subgraph containing*

$$\{v_5, c_\alpha, n_\alpha, c_\beta, o_x, o_{2'}\} \quad (957)$$

and possess the same stereochemical label at c_α . Then either both satisfy the principal stereochemical target predicate or neither does.

Proof. The principal target predicate depends only on the local relations

$$v_5 - c_\alpha, \quad c_\alpha - n_\alpha, \quad c_\alpha - c_\beta, \quad c_\beta = o_x, \quad c_\beta - o_{2'}, \quad (958)$$

together with $\chi(c_\alpha)$. All these data agree by hypothesis. $\square$

D.8 Witness criterion for target-family reachability

Proposition D.13 (Finite witness criterion). *Let*

$$S_0 \xrightarrow{e_1} S_1 \xrightarrow{e_2} \dots \xrightarrow{e_n} S_n \quad (959)$$

be a finite sequence of elementary cage-constrained transitions.

If

$$S_n \in \mathfrak{T} \quad (960)$$

for a declared target family $\mathfrak{T}$, then

$$\exists T \in \mathfrak{T} \text{ such that } \text{Hom}_{\mathbf{Reach}_c}(S_0, T) \neq \emptyset. \quad (961)$$

Proof. The free-category composite

$$e_n \circ \dots \circ e_1 \quad (962)$$

is a morphism

$$S_0 \longrightarrow S_n. \quad (963)$$

Take $T = S_n$. $\square$

D.9 Model-theoretic formulation of conditional non-vacuity

The model-theoretic statement associated with the main theorem requires a distinction between logical consequence and satisfiability.

Let

$$\mathsf{T}_{\text{base}} \quad (964)$$

denote the inherited formalism together with the state, reaction, cage, and reachability definitions.

Let

$$\mathsf{H}_{\text{fam}} \quad (965)$$

denote one of the complete family-level hypothesis packages used in the main theorem, and define

$$\mathsf{T}_{\text{CCR}} := \mathsf{T}_{\text{base}} \cup \mathsf{H}_{\text{fam}}. \quad (966)$$

Let

$$\text{ReachTarget} \quad (967)$$

denote the sentence expressing the corresponding target-family reachability conclusion.

Proposition D.14 (Conditional satisfiability transfer). *Suppose the main existence theorem has been formalized as*

$$\mathsf{T}_{\text{CCR}} \models \text{ReachTarget}. \quad (968)$$

If

$$\text{Mod}(\mathsf{T}_{\text{CCR}}) \neq \emptyset, \quad (969)$$

then

$$\boxed{\text{Mod}(\mathsf{T}_{\text{CCR}} \cup \{\text{ReachTarget}\}) = \text{Mod}(\mathsf{T}_{\text{CCR}}) \neq \emptyset.} \quad (970)$$

Proof. Every model of T_{CCR} satisfies ReachTarget by Equation (968).

Therefore adjoining the already entailed target sentence removes no models:

$$\text{Mod}(\mathsf{T}_{\text{CCR}} \cup \{\text{ReachTarget}\}) = \text{Mod}(\mathsf{T}_{\text{CCR}}). \quad (971)$$

The latter class is nonempty by hypothesis. $\square$

Remark D.15 (Logical consequence versus empirical satisfiability). The existence theorem establishes the implication from the declared realization hypotheses to target reachability.

It does not, by itself, establish

$$\text{Mod}(\mathsf{T}_{\text{CCR}}) \neq \emptyset. \quad (972)$$

That additional statement requires joint satisfiability of the realization hypotheses, which is precisely the role

of the computational and experimental certification program of Section 11.

E Alternative Realization Transports and Path-Space Extensions

This appendix records technical extensions of the alternative-realization theory developed in Section 10.

The principal existence theorems require only nonemptiness of a suitable hom-set. The constructions below retain additional information concerning realization indexing, reaction-word multiplicity, path length, realization-specific path cost, and compatibility among distinct transport operations.

E.1 Explicit realization transports

For the reference $C6 \rightarrow C5$ realization, let

$$U_{\text{rxn}}^{6 \rightarrow 5} \quad (973)$$

be the completed local reaction support.

For the dual $C5 \rightarrow C6$ realization, let

$$U_{\text{rxn}}^{5 \rightarrow 6} \quad (974)$$

be the corresponding transported support.

The dual-cipher support identification is

$$\Sigma_{56} : U_{\text{rxn}}^{6 \rightarrow 5} \longrightarrow U_{\text{rxn}}^{5 \rightarrow 6}, \quad (975)$$

with

$$\begin{aligned} \Sigma_{56}(v_6) &= v_5, & \Sigma_{56}(v_5) &= v_6, \\ \Sigma_{56}(o_6) &= o_5, & \Sigma_{56}(c_\alpha) &= c_\alpha^{(5)}, \\ \Sigma_{56}(c_\beta) &= c_\beta^{(5)}, & \Sigma_{56}(o_\beta) &= o_\beta^{(5)}. \end{aligned} \quad (976)$$

Shared adenosine-side labels are fixed when their realization roles are unchanged:

$$\Sigma_{56}(o_{2'}) = o_{2'}, \quad \Sigma_{56}(p) = p. \quad (977)$$

For every reference rule p_i , the formally transported rule is

$$p_i^{(5)} = (\Sigma_{56})_* p_i. \quad (978)$$

The corresponding canonical dual word is

$$\Phi_{\text{can}}^{5 \rightarrow 6} = p_{\text{tr}}^{(5)} \circ p_{\text{am}}^{(5)} \circ p_{\text{carb}}^{(5)} \circ p_{\text{epox}}^{(5)} \circ p_{\text{unsat}}^{(5)} \circ p_{\text{cap}}^{(5)}. \quad (979)$$

Equation (978) is a graph-theoretic transport. Cage-constrained transport additionally requires the hypotheses of Theorem 10.7.

For an adenine-anchor change

$$C2 \longrightarrow N6, \quad (980)$$

the chemical support map is

$$\text{id}_{U_{\text{rxn}}} : U_{\text{rxn}}^{C2} \longrightarrow U_{\text{rxn}}^{N6} \quad (981)$$

whenever Hypothesis 10.8 holds.

Likewise, for $\Lambda, \Lambda' \in \mathcal{L}$, remote-substitution transport acts chemically as

$$\text{id}_{U_{\text{rxn}}} : U_{\text{rxn}}^\Lambda \longrightarrow U_{\text{rxn}}^{\Lambda'} \quad (982)$$

under local chemical concordance.

In both cases the chemical support map may be the identity while the corresponding cage spaces differ.

E.2 Discrete realization family

The principal discrete realization parameters are:

$$\Lambda \in \{\{6, 12\}, \{3, 6, 12\}, \{3, 6, 9, 12\}\}, \quad (983)$$

$$\eta_A \in \{C2, N6\}, \quad (984)$$

and

$$d_{\text{dc}} \in \{6 \rightarrow 5, 5 \rightarrow 6\}. \quad (985)$$

Define

$$\mathcal{P}_{\text{disc}} := \mathcal{L} \times \{C2, N6\} \times \{6 \rightarrow 5, 5 \rightarrow 6\}. \quad (986)$$

Hence

$$\#\mathcal{P}_{\text{disc}} = 3 \cdot 2 \cdot 2 = 12. \quad (987)$$

For $\mathbf{p} \in \mathcal{P}_{\text{disc}}$, define the reachability indicator

$$a(\mathbf{p}) = \begin{cases} 1, & \exists T_\star^\mathbf{p} \in \mathfrak{T}_\star^\mathbf{p} \text{ such that } S_0^\mathbf{p} \preceq_C^\mathbf{p} T_\star^\mathbf{p}, \\ 0, & \text{otherwise.} \end{cases} \quad (988)$$

The admissible discrete realization subset is

$$\mathcal{P}_{\text{adm}} = \{\mathbf{p} \in \mathcal{P}_{\text{disc}} : a(\mathbf{p}) = 1\}. \quad (989)$$

The mathematical framework does not assert

$$\mathcal{P}_{\text{adm}} = \mathcal{P}_{\text{disc}}. \quad (990)$$

Each realization point has its own chemical and geometric certification problem.

E.3 Path length

Let

$$f = e_n \cdots e_1 \quad (991)$$

be a nonidentity morphism of a free reaction category.

Define

$$\ell(f) := n. \quad (992)$$

For an identity morphism,

$$\ell(1_S) = 0. \quad (993)$$

For composable morphisms

$$f : S \longrightarrow T, \quad g : T \longrightarrow U, \quad (994)$$

one has

$$\ell(g \circ f) = \ell(g) + \ell(f). \quad (995)$$

Thus path length records the number of elementary transitions in the chosen reaction grammar. It is grammar dependent rather than an intrinsic physical reaction time.

E.4 Length-bounded path multiplicity

For $L \in \mathbb{N}_0$, define

$$\text{Hom}^{\leq L}(S, T) := \{f \in \text{Hom}(S, T) : \ell(f) \leq L\}. \quad (996)$$

Proposition E.1 (Finite bounded-length path count).

Suppose the relevant transition quiver contains finitely many generating edges.

Then for every finite L and every pair S, T ,

$$\#\text{Hom}^{\leq L}(S, T) < \infty. \quad (997)$$

Proof. Let $M < \infty$ be the number of generating edges. There are at most

$$1 + M + M^2 + \cdots + M^L \quad (998)$$

formal edge words of length at most L .

The composable words with prescribed source and target form a subset. $\square$

For a realization $\mathbf{p}$, define the length-bounded target-path set

$$\mathcal{W}_*^{\leq L}(\mathbf{p}) := \coprod_{T \in \mathfrak{T}_*^{\mathbf{p}}} \text{Hom}_{\text{Reach}_{\mathbf{C}}^{\mathbf{p}}}^{\leq L}(S_0^{\mathbf{p}}, T). \quad (999)$$

Whenever the relevant transition quiver is finite,

$$N_{\text{path}}^{\leq L}(\mathbf{p}) := \#\mathcal{W}_*^{\leq L}(\mathbf{p}) \quad (1000)$$

is finite.

This provides a finite search space after both the rule grammar and the maximum path length have been prospectively bounded.

E.5 Length-minimal witnesses

Suppose

$$\text{Hom}(S, T) \neq \emptyset. \quad (1001)$$

Define

$$\ell_{\min}(S, T) := \min \{\ell(f) : f \in \text{Hom}(S, T)\}. \quad (1002)$$

The minimum exists because the nonempty set of path lengths is a subset of $\mathbb{N}_0$.

Definition E.2 (Length-minimal witness). A morphism

$$f : S \longrightarrow T \quad (1003)$$

is a *length-minimal witness* when

$$\ell(f) = \ell_{\min}(S, T). \quad (1004)$$

The canonical witness need not be length minimal. For example, a newly admitted direct generator

$$q_{\beta} : S_1 \longrightarrow S_4 \quad (1005)$$

would shorten the canonical three-generator carbonyl factorization without affecting the validity of the longer existence witness.

E.6 Realization-specific path cost

The free reaction category distinguishes reaction words but does not assign them physical preference.

A realization may therefore introduce an additional functional

$$\mathcal{A}_{\text{phys}} : \text{Mor}(\mathbf{Reach}_{\mathbf{C}}^{\mathbf{p}}) \longrightarrow [0, \infty]. \quad (1006)$$

When activation free energies have been independently assigned to the elementary transitions, possible examples include

$$\mathcal{A}_{\max}(f) = \max_i \Delta G_i^{\ddagger} \quad (1007)$$

or

$$\mathcal{A}_{\Sigma}(f) = \sum_i w_i \Delta G_i^{\ddagger}, \quad w_i \geq 0. \quad (1008)$$

One may then define a cost-minimizing witness by

$$f_{\star} \in \arg \min_{f \in \text{Hom}(S, T)} \mathcal{A}_{\text{phys}}(f) \quad (1009)$$

when the minimum exists.

Neither $\mathcal{A}_{\text{phys}}$ nor minimization of it is a premise of the principal existence theorem.

E.7 Transport squares

For fixed Λ , consider the four realization classes

$$\mathcal{R}_{\Lambda, C2}^{6 \rightarrow 5}, \quad \mathcal{R}_{\Lambda, N6}^{6 \rightarrow 5}, \quad \mathcal{R}_{\Lambda, C2}^{5 \rightarrow 6}, \quad \mathcal{R}_{\Lambda, N6}^{5 \rightarrow 6}. \quad (1010)$$

Let

$$\mathfrak{A} \quad (1011)$$

denote an anchor-transport functor where defined, and let

$$\mathfrak{D} \quad (1012)$$

denote dual-cipher transport.

Schematically,

$$\begin{array}{ccc} \mathcal{R}_{\Lambda, C2}^{6 \rightarrow 5} & \xrightarrow{\mathfrak{A}} & \mathcal{R}_{\Lambda, N6}^{6 \rightarrow 5} \\ \mathfrak{D} \downarrow & & \downarrow \mathfrak{D} \\ \mathcal{R}_{\Lambda, C2}^{5 \rightarrow 6} & \xrightarrow{\mathfrak{A}} & \mathcal{R}_{\Lambda, N6}^{5 \rightarrow 6}. \end{array} \quad (1013)$$

If the journal class does not provide the `CD` environment, Equation (1013) may be replaced by an equivalent `array` or `tikzcd` representation during final typesetting.

Definition E.3 (Transport-concordant realization square). The realization square is *transport concordant* on a selected local reaction category when both composite transports are defined and

$$\boxed{\mathfrak{D} \circ \mathfrak{A} = \mathfrak{A} \circ \mathfrak{D}} \quad (1014)$$

on that category.

This condition is stronger than required by the principal existence theorem.

It asserts that anchor change followed by dual-cipher transport gives the same transported local reaction data as dual-cipher transport followed by anchor change.

E.8 Remote-substitution direction

The substitution family supplies an additional realization direction

$$\Lambda_2 \longrightarrow \Lambda_3 \longrightarrow \Lambda_4. \quad (1015)$$

On the completed chemical support, the corresponding map is the identity under exact local chemical concordance:

$$\text{id}_{U_{\text{rxn}}}. \quad (1016)$$

At the geometric level, each arrow in Equation (1015) requires its own candidate transported lifts and constraint-deviation certificate.

Thus the full realization family is more accurately viewed as a finite discrete base carrying realization-indexed local reaction categories, rather than as a single category with automatically equivalent geometries.

E.9 Abstract nonunique-solution principle

Theorem E.4 (Nonunique-solution reachability principle). Let $\mathcal{P}$ be a family of molecular realization parameters and let $\mathfrak{T}_*^{\mathbf{P}}$ be their corresponding target classes. Suppose there exists at least one

$$\mathbf{p}_0 \in \mathcal{P} \quad (1017)$$

and at least one morphism

$$f_0 : S_0^{\mathbf{p}_0} \longrightarrow T_*^{\mathbf{p}_0}, \quad T_*^{\mathbf{p}_0} \in \mathfrak{T}_*^{\mathbf{p}_0}. \quad (1018)$$

Then target existence is established for $\mathbf{p}_0$ independently of whether:

1. additional reaction words exist in the same realization;
2. additional molecular realizations reach corresponding targets;
3. the complete terminal coproduct state is unique; or
4. f_0 is length minimal or cost optimal.

Proof. Target existence for $\mathbf{p}_0$ is exactly the statement that the corresponding target hom-set is nonempty. The listed uniqueness and optimization properties are strictly additional conditions and are not required for nonemptiness. $\square$

E.10 Path-space summary

The principal hierarchy is

$$\begin{array}{c} \text{Hom}(S, T) \neq \emptyset \\ \Downarrow \\ \text{target reachability} \\ \# \text{Hom}(S, T) \geq 2 \\ \Downarrow \\ \text{reaction-word nonuniqueness} \\ \# \mathcal{R}(T_*) \geq 2 \\ \Downarrow \\ \text{realization nonuniqueness.} \end{array} \quad (1019)$$

Path length and physical cost refine this structure but do not replace the underlying existence criterion.

F Source, Notation, and Claim Concordance

This appendix records the logical origin of the structures used in the paper and collects the principal notation after

the revisions of Sections 2–11.

Its purpose is to distinguish inherited mathematical structure, motivating molecular architecture, realization-specific hypotheses, present-paper definitions, and proved consequences.

F.1 Logical source classes

Five source classes are distinguished.

Inherited mathematical structure.

Definitions, classification results, locant data, attachment data, and other mathematical objects taken as fixed input from the prior Chrysene Formalism.

Motivating molecular architecture.

Substituted-chrysene, stacked, tethered, nucleoside-linked, or related molecular architectures used to define the realization class.

Present-paper definition.

Reaction states, persistent atom maps, graph-rewrite rules, cage-admissible configuration spaces, reaction categories, target classes, and certification objects introduced in this work.

Realization hypothesis.

A chemical, geometric, stereochemical, energetic, or physical condition that must be supplied for a particular theorem application.

Present-paper theorem or derived consequence.

A mathematical conclusion proved from the declared definitions and hypotheses.

Bibliographic citations associated with inherited or motivating material are supplied by the corresponding main-text source statements. The logical classification in this appendix does not itself convert a documentary source into proof of a realization hypothesis.

F.2 Structural and theorem-source concordance

The principal objects have the following logical roles.

$\mathcal{C}_{\text{chr}}$.

Inherited mathematical structure. The fixed canonical chrysene molecular anchor.

$\mathcal{S}_{\text{pri}}, \mathcal{S}_{\text{dual}}$.

Inherited mathematical structure. The primary and dual locant sets used by the realization theory.

$\delta_{\text{dc}}, \sigma_{\text{dc}}$.

Inherited mathematical structure. Locant-level primary–dual pairing data. These maps are not identified with Euclidean symmetry of an instantiated molecule.

∂G_{chr} and $C6/C5$ adjacency.

Inherited mathematical structure together with its direct local consequence used by the present reaction construction.

τ and π_{ℓ} .

Inherited directional attachment data together with the present realization’s local geometric orientation scalar.

Substituted and stacked molecular architectures.

Motivating molecular architecture. They motivate the realization family but do not certify chemical reachability.

$S = (G, \iota, q, r, s, \chi, \rho, \mathcal{K})$.

Present-paper definition. The typed molecular state carrying chemical and cage data.

$\mathcal{P}, \text{Pat}(p), \text{Act}(p)$.

Present-paper definitions. The local reaction grammar and its pattern/action supports.

$U_6, U_{\text{rxn}}, C(S)$.

Present-paper definitions. Respectively the structural reaction neighborhood, completed chemical rule support, and geometric cage support.

$\text{Lift}_{\mathcal{C}}(p; S, T)$.

Present-paper definition. The set of cage-compatible geometric lifts of a chemically admissible rewrite.

Chem.

Present-paper definition. The free category generated by chemically admissible elementary transitions.

Reach $_{\mathcal{C}}$.

Present-paper definition. The free category generated by cage-liftable chemical transitions.

Local transformation invariance.

Present-paper theorem. Exact chemical context extension combined with candidate geometric transport and the inequality $\Delta_{\mathcal{F}}^A < m_{\text{min}}$.

Φ_{can} .

Present-paper construction. A six-generator explicit witness candidate for the reference transformation.

Reference and family-level existence.

Present-paper theorems. Nonemptiness of the relevant target hom-sets under the declared hypothesis packages.

Stereochemical selection.

Present-paper theorem layer. The conclusion $\chi(c_{\alpha}) = \chi_{\star}$ under strong cage selection and stereospecific reaction hypotheses.

P_{β}^{epox} and P_{β}^{hyd} .

Present-paper constructions. Alternative reaction words having the same intended carbonyl endpoint.

Σ_{56} .

Present-paper realization transport constructed from inherited dual-cipher locant data. Its physical application requires independent cage compatibility.

$C2 \rightarrow N6$ anchor transport.

Present-paper realization transport. Chemical support may remain fixed while cage geometry changes.

$G_0, \dots, G_7$.

Present-paper certification architecture. These gates test whether a specified realization supports the hypotheses used by the conditional theorems.

F.3 Notation concordance

The principal notation used after revision is:

$\mathbb{A}$ Persistent closed reaction atom universe.

$\mathcal{L}$ Substitution family $\{\{6, 12\}, \{3, 6, 12\}, \{3, 6, 9, 12\}\}$.

Λ One chrysene substitution context.

η_A Adenine attachment parameter, with $C2$ the reference value.

U_6 Structural $C5/C6$ -centered reaction neighborhood.

U_{rxn} Completed local chemical pattern support,

$$U_{\text{rxn}} = U_6 \cup \bigcup_{p \in \mathcal{P}_6} \text{Pat}(p).$$

$C(S)$

Finite geometric cage support of state S .

$\mathcal{K}_C(S)$

Projected cage-admissible set on $C(S)$.

$\mathcal{K}(S)$

Full-state cage-admissible configuration set.

$\mathcal{X}_p$ Ambient transition configuration space for rule p .

$\mathcal{C}_p$ Hard-constrained transition domain for rule p .

$\text{Lift}_C(p; S, T)$

Geometric lift space.

Chem

Free chemical path category.

Reach_C

Free cage-constrained reaction category.

Reach_A^{6→5}

Reference $C6 \rightarrow C5$, realization-indexed cage category.

Reach_A^{5→6}

Dual $C5 \rightarrow C6$ realization category.

$\mathfrak{T}_{\text{conn}}^\Lambda$

Connectivity target class without a specified c_α configuration.

$\mathfrak{T}_*^\Lambda$

Stereochemically specified target class.

Φ_{can}

Canonical six-generator witness.

P_β^{epox}

Canonical unsaturation–oxygenation–carbonyl composite.

P_β^{hyd}

Alternative hydroxylation–oxidation carbonyl composite.

χ_*

Selected absolute configuration at c_α .

χ_L

Absolute configuration corresponding to the intended L-series assignment after full stereochemical convention is specified.

Σ_{56} Local support transport from the $C6 \rightarrow C5$ realization to the $C5 \rightarrow C6$ realization.

m_{min}

Uniform positive margin over the designated hard inequality constraints of the selected reference path.

$\Delta_{\mathcal{F}}^\Lambda$

Maximum transported deviation over the augmented hard-constraint family.

δ_χ

Stereochemical branch margin.

ζ_χ

Oriented stereochemical attack scalar $\langle u_{\text{att}}, e_3 \rangle$.

H_{conn}

Reference connectivity-level hypothesis package.

H_{ref}

Reference stereochemical hypothesis package.

$H_{\text{loc}}^{\text{conn}}$

Connectivity-level family transport package.

H_{loc}^χ

Stereochemical family transport package.

$H_{\text{fam}}^{\text{conn}}, H_{\text{fam}}^\chi$

Complete family-level theorem packages.

$G_0, \dots, G_7$

Canonical realization-certification gates.

G'_4

Alternative hydroxylation–oxidation carbonyl certification gate.

$\nu(H)$

Three-valued realization status in $\{\text{U}, \text{C}, \text{F}\}$.

F.4 Claim-status concordance

The manuscript uses four distinct logical forms.

A *definition* introduces a mathematical object:

$$D := \text{specified structure.} \quad (1020)$$

A *realization hypothesis* asserts a condition to be supplied by a particular molecular model:

$$\text{H.} \quad (1021)$$

A *conditional theorem* has the form

$$\text{H} \implies P. \quad (1022)$$

A *realization certificate* supplies evidence that a specified molecular realization satisfies a member of H .

Thus

$\text{definition} \neq \text{realization hypothesis} \neq \text{conditional theorem} \neq \text{physical realization}$

(1023)

F.5 Documentary and mechanistic boundary

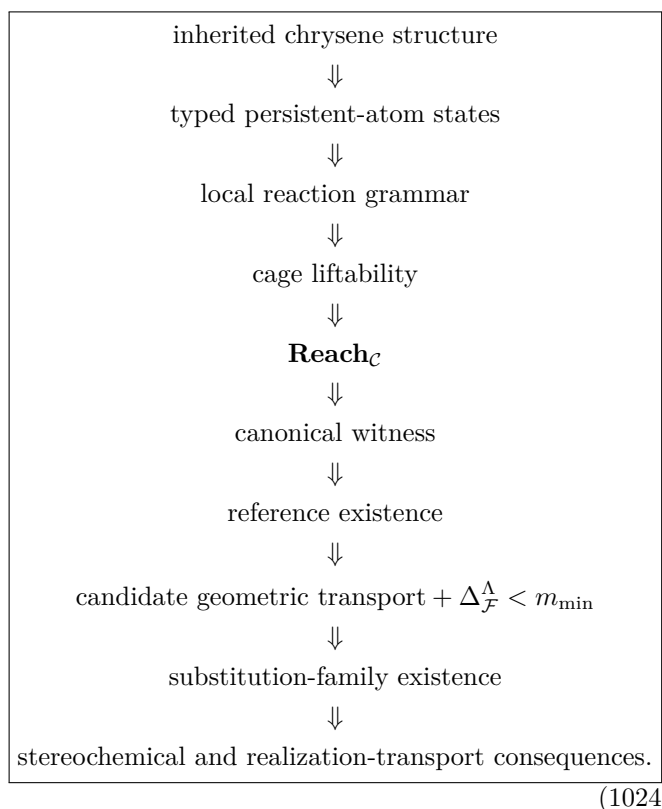
Patent or other molecular-architecture disclosures are documentary sources for motivating realization classes. Patent status, claim scope, or disclosure of a molecular architecture is not used as proof of a reaction mechanism or theorem hypothesis.

Likewise, the inherited Chrysene Formalism supplies the fixed molecular and locant structures listed above. Chemical transformations introduced in the present manuscript belong to the new realization layer rather than following automatically from the foundational theory.

These distinctions are governed globally by Convention 2.2.

F.6 Theorem dependency concordance

The principal dependency structure is



The dependency direction is one-way. Failure to certify one physical realization does not alter the formal definitions or the conditional theorem, and failure of one reaction word does not imply an empty target hom-set when another admissible witness remains.

F.7 Final logical boundary

The complete manuscript distinguishes:

I. Mathematical implication
$H_\Theta \implies P,$
II. Realization question
Does a specified molecular system satisfy H_Θ ?
III. Physical-path question
Which certified reaction word, if any, is observed?

(1025)

Assertion I is the object of mathematical proof. Assertions II and III require the certification framework of Section 11 and Appendix G.

G Computational and Experimental Certification Protocols

This appendix provides the detailed implementation layer for the certification architecture of Section 11.

The protocols below do not replace the mathematical hypotheses. Their role is to define prospective evidence classes capable of assigning the realization status

$$\nu(H) \in \{U, C, F\} \quad (1026)$$

to the hypotheses required by a selected theorem branch.

Numerical thresholds are intentionally not fixed by the abstract theory. Whenever a gate requires an energetic, geometric, population, or selectivity cutoff, the threshold must be declared prospectively for the realization being tested.

G.1 Prospective certification design

For every realization hypothesis H_j , a certification protocol should specify:

$$\mathcal{C}_j = (H_j, M_j, D_j, A_j, R_j), \quad (1027)$$

where M_j is the method, D_j the evidence object, A_j the acceptance predicate, and R_j the associated uncertainty and validity statement.

The acceptance criterion should be fixed before the evidence is interpreted whenever practicable.

A conclusion is recorded as:

$$\nu(H_j) = \begin{cases} U, & \text{insufficient evidence,} \\ C, & A_j(D_j) = 1, \\ F, & \text{the declared disqualifying criterion is satisfied.} \end{cases} \quad (1028)$$

G.2 Method-refinement hierarchy

Different gates require different physical information. A single computational method need not be appropriate for every gate.

A realization may therefore specify a refinement hierarchy

$$\mathcal{M}_0 \prec \mathcal{M}_1 \prec \cdots \prec \mathcal{M}_K, \quad (1029)$$

where the ordering denotes increasing resolution or physical scope for the observable being tested.

A representative hierarchy may contain:

$\mathcal{M}_0$: rapid conformational or semiempirical screening,

$\mathcal{M}_1$: dispersion-aware electronic-structure optimization,

$\mathcal{M}_2$: higher-resolution single-point energetic refinement,

$\mathcal{M}_3$: excited-state, spin-flip, or multireference treatment when required

$\mathcal{M}_4$: explicit-environment or QM/MM refinement,

$\mathcal{M}_5$: experimental structural, kinetic, or spectroscopic evidence.

(1030)

The hierarchy is illustrative rather than mandatory. The selected method must be appropriate to the physical observable being certified.

Definition G.1 (Method-stable certification). A certification decision is *method stable* over a declared method family when every method above a prospectively specified minimum resolution preserves the qualitative gate decision.

A conclusion that changes from accepted to rejected under modest method or environmental refinement should be reported as model sensitive rather than robustly certified.

G.3 Uncertainty-aware thresholding

For a computed scalar observable

$$Y, \quad (1031)$$

associate an uncertainty interval

$$I_Y = [Y^-, Y^+]. \quad (1032)$$

If a gate requires

$$Y \leq Y_{\max}, \quad (1033)$$

a conservative certificate may require

$$Y^+ \leq Y_{\max}. \quad (1034)$$

If the gate requires

$$Y \geq Y_{\min}, \quad (1035)$$

a conservative criterion is

$$Y^- \geq Y_{\min}. \quad (1036)$$

A point estimate whose uncertainty interval crosses the declared decision boundary is not treated as a robust threshold certificate.

G.4 Ensemble-level certification

The cage is a conformational system rather than a single rigid structure.

Let

$$\mu_S \quad (1037)$$

be a normalized ensemble weight or probability measure on $\mathcal{K}(S)$.

For a gate-admissible subset

$$\mathcal{A}_G \subseteq \mathcal{K}(S), \quad (1038)$$

define

$$P_G := \mu_S(\mathcal{A}_G). \quad (1039)$$

An existence-level criterion may require only

$$P_G > 0, \quad (1040)$$

whereas a practical realization criterion may require

$$P_G \geq P_{\min} \quad (1041)$$

for a prospectively specified $P_{\min}$.

These are different claims:

$$P_G > 0 \quad (1042)$$

supports ensemble-level existence, whereas a substantial population supports a stronger accessibility interpretation.

G.5 Gate G_0 : structural and cage realization

Construct a conformational ensemble

$$\mathcal{E}_0 = \{x_1, \dots, x_M\} \subseteq \text{Conf}(\mathbb{A}) \quad (1043)$$

using a declared structural-sampling protocol.

Candidate evidence-generating methods may include molecular dynamics, enhanced sampling, semiempirical or tight-binding optimization, electronic-structure refinement, or experimentally restrained structural modeling.

For each configuration, evaluate the cage observables required by the selected realization, including as applicable

$$d_\pi, \quad s_\pi, \quad \Theta_\pi, \quad d_{v_5 c_\alpha}, \quad d_{c_\beta o_{2'}}, \quad (1044)$$

together with the complete state-constraint family of Appendix C.

The minimum existence-level structural criterion is

$$\exists x \in \mathcal{E}_0 \text{ such that } x \in \mathcal{K}(S_0). \quad (1045)$$

An ensemble-level realization may instead require

$$P_{G_0} \geq P_{\min}^{(0)}. \quad (1046)$$

A structural certificate should report the sampling method, ensemble size or effective sample size, convergence assessment, cage-observable distributions, and the population satisfying the declared hard constraints.

G.6 Gate G_1 : capture

The capture gate corresponds to

$$p_{\text{cap}} : \text{C6} - \text{O} - \text{C}_\alpha \rightsquigarrow \text{C5} - \text{C}_\alpha. \quad (1047)$$

The geometric part requires configurations satisfying the declared capture windows

$$d_{\text{cap}} \in I_{\text{cap}}^d, \quad \theta_{\text{cap}} \in I_{\text{cap}}^\theta, \quad (1048)$$

together with all persistent cage constraints.

The electronic component should determine whether at least one declared electronic route connects the selected reactant state to a state compatible with the net atom-mapped rewrite.

A prospective computational sequence may be organized as

$$\begin{array}{l} \text{ground-state characterization} \\ \Downarrow \\ \text{vertical excitation or activation-state analysis} \\ \Downarrow \\ \text{state-character assignment} \\ \Downarrow \\ \text{reactive-coordinate relaxation} \\ \Downarrow \\ \text{transition-path or surface-crossing analysis.} \end{array} \quad (1049)$$

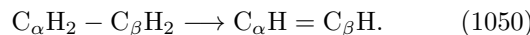
State characterization may use transition densities, natural transition orbitals, spin densities, bond-order observables, or other method-appropriate diagnostics.

If the selected single-reference description becomes qualitatively unstable along the reactive coordinate, the certificate should be refined by an electronic-structure treatment appropriate to that failure mode.

Gate G_1 is certified only when both the capture geometry and the declared electronic pathway satisfy their prospective acceptance criteria.

G.7 Gate G_2 : local unsaturation

The canonical unsaturation is



The calculation must include the explicitly selected hydrogen acceptor, oxidant, or redox partner required by the balanced completion of p_{unsat} .

Atom mapping must verify the terminal states of

$$h_{\alpha,2}, \quad h_{\beta,2}. \quad (1051)$$

Relevant realization observables may include

$$\Delta G_{\text{unsat}} \quad (1052)$$

and, where a transition-state description is meaningful,

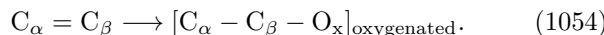
$$\Delta G_{\text{unsat}}^\ddagger. \quad (1053)$$

Gate G_2 is passed when a fully balanced path from S_1 to S_2 is identified and satisfies the prospectively declared energetic and chemical-admissibility criteria.

G.8 Gate G_3 : oxygen addition

The oxygen donor must be specified explicitly and the atom map must identify the persistent oxygen o_x .

The intended transformation is



The analysis should distinguish the intended pathway from declared competing channels such as alternative aromatic oxidation, phosphate oxidation or cleavage, peroxide formation, or other unproductive oxygen-transfer products.

When activation barriers are used, define

$$\Delta G_{\text{epox}}^\ddagger \quad (1055)$$

for the intended route and

$$\Delta G_{j,\text{comp}}^\ddagger \quad (1056)$$

for competing channel j .

Then

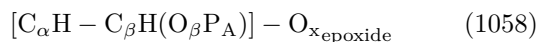
$$\Delta \Delta G_{\text{epox},j}^\ddagger = \Delta G_{j,\text{comp}}^\ddagger - \Delta G_{\text{epox}}^\ddagger \quad (1057)$$

is one possible selectivity observable.

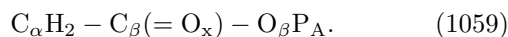
The gate criterion should be stated prospectively in terms of the required oxygen provenance, reaction-path continuity, and competing channel tolerance.

G.9 Gate G_4 : canonical carbonyl formation

The canonical gate requires



to reach



The defining requirement is both carbonyl formation and retention of



A computational certificate should characterize, as applicable: the oxygenated reactant basin, hydrogen-transfer coordinate, developing $C_\beta = O_x$ bond, retained $C_\beta - O_\beta$ bond, and a transition structure or minimum-energy path connecting the declared endpoints.

When a well-defined transition state exists, an intrinsic reaction coordinate or equivalent path-following method should be used to verify connection to the intended reactant and product basins.

Define

$$R_P = \begin{cases} 1, & \text{the certified route retains } C_\beta - O_\beta - P_A, \\ 0, & \text{otherwise.} \end{cases} \quad (1061)$$

The canonical gate requires

$$R_P = 1. \quad (1062)$$

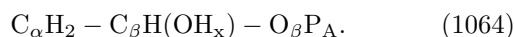
If the selected route instead loses the phosphate-containing linkage before carbonyl formation, the canonical G_4 branch is rejected for that realization.

G.10 Alternative gate G'_4 : hydroxylation-oxidation

The alternative carbonyl factorization is

$$P_\beta^{\text{hyd}} = q_{\text{ox}} \circ q_{\text{hyd}}. \quad (1063)$$

The proposed intermediate is



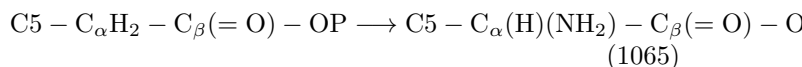
The certificate should determine whether:

1. the hydroxylated state exists as a meaningful minimum or dynamically populated intermediate;
2. the $C_\beta - O_\beta - P_A$ linkage is retained;
3. the mapped oxygen o_x becomes the carbonyl oxygen during oxidation; and
4. dominant fragmentation or competing oxidation does not violate the declared gate criterion.

Gate G'_4 certifies the complete alternative $S_1 \rightarrow S_4$ carbonyl branch. It is not merely an alternative final rearrangement step appended to G_2 and G_3 .

G.11 Gate G_5 : amino installation

The principal connectivity change is



The nitrogen source must be represented explicitly in the balanced reaction universe.

For each declared amination pathway, the certificate should verify: persistent atom transfer of n_α , valid removal of $h_{\alpha, \text{am}}$, formation of $c_\alpha - n_\alpha$, preservation of the C_β -carbonyl-containing unit, and preservation of the chrysene anchor.

Where distinguishable attack faces exist, both should be evaluated unless one is excluded geometrically by the strong stereochemical gate.

Gate G_5 certifies amination connectivity only.

G.12 Gate G_6 : stereochemical selection

Two different certification targets must be distinguished.

For the strong geometric theorem, require

$$\mathcal{U}_N \cap \mathcal{A}_{\chi_*} \neq \emptyset \quad (1066)$$

and

$$\mathcal{U}_N \cap \mathcal{A}_{\chi_{\text{opp}}} = \emptyset. \quad (1067)$$

This is the certification target corresponding to deterministic branch selection in the mathematical theorem.

For an energetic realization, define

$$\Delta\Delta G_\chi^\ddagger = \Delta G_{\text{opp}}^\ddagger - \Delta G_\star^\ddagger. \quad (1068)$$

A prospective energetic gate may require

$$\Delta\Delta G_\chi^\ddagger \geq \Delta\Delta G_{\text{min}}^\ddagger. \quad (1069)$$

Under a stated transition-state model, a branch ratio may scale with

$$\exp\left(\frac{\Delta\Delta G_\chi^\ddagger}{RT}\right), \quad (1070)$$

but translation from a computed barrier difference to an experimental enantiomeric excess requires an explicitly declared kinetic model.

After product structure is obtained, the stereochemical certificate must also establish the complete substituent ordering at c_α .

Let

$$\text{CIP}(c_\alpha) \quad (1071)$$

denote the resulting priority assignment.

The complete L-series certificate contains:

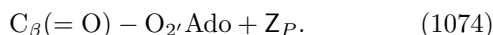
$$\begin{aligned}
 &\text{product structure} \\
 &+ \text{CIP ordering} \\
 &+ \text{absolute } R/S \text{ assignment} \\
 &+ \text{explicit L/D convention} \\
 &\Downarrow \\
 &\chi_{\star} = \chi_L.
 \end{aligned} \tag{1072}$$

G.13 Gate G_7 : terminal 2'-O acyl transfer

The intended transformation is



to



The cage analysis should evaluate

$$d_{c_{\beta}o_{2'}}, \quad \theta_{acyl}, \tag{1075}$$

together with any declared proton-transfer geometry.

The reaction calculation must distinguish attack at C_{β} from plausible competing processes centered at phosphorus or other nucleophilic sites.

If barriers are used, define

$$\Delta G_{acyl}^{\ddagger} \tag{1076}$$

for the intended acyl transfer and

$$\Delta G_{P,j}^{\ddagger} \tag{1077}$$

for the j -th competing phosphorus-centered process.

Then

$$\Delta \Delta G_{tr,j}^{\ddagger} = \Delta G_{P,j}^{\ddagger} - \Delta G_{acyl}^{\ddagger} \tag{1078}$$

is one possible transfer-selectivity observable.

The gate additionally requires: formation of the persistent $c_{\beta} - o_{2'}$ bond, retention of $c_{\beta} = O$, and placement of the departing phosphate-containing atoms in an allowed terminal state.

G.14 Experimental atom-provenance certification

The persistent atom map gives mechanism-discriminating isotope predictions.

For the canonical oxygenation/carbonyl route,

$$o_{\text{carbonyl}} = o_x. \tag{1079}$$

If the donor-derived oxygen is isotopically labeled,

$$^{18}O_x, \tag{1080}$$

the canonical path predicts

$$c_{\beta} = ^{18}O \tag{1081}$$

in the terminal carbonyl.

By contrast, labeling the original tether oxygen o_6 does not label the C_{β} carbonyl under this canonical atom map.

Define the provenance observable

$$I_{\beta} = \begin{cases} 1, & ^{18}O \text{ is observed at the mapped } C_{\beta} \text{ carbonyl,} \\ 0, & \text{otherwise.} \end{cases} \tag{1082}$$

The analytical method must be capable of assigning the isotope to the carbonyl position rather than merely detecting isotope incorporation somewhere in the product.

G.15 Experimental connectivity and regioisomer certification

The principal target requires

$$\bar{b}(v_5, c_{\alpha}) = 1. \tag{1083}$$

Experimental evidence should therefore distinguish $C_5 - C_{\alpha}$ attachment from alternative chrysene-locant connectivity.

Evidence classes may include, as appropriate, NMR connectivity or correlation measurements, isotope-assisted structural assignment, high-resolution mass-fragmentation support, or direct structural methods.

The theorem requires the connectivity assignment rather than one particular instrument.

Terminal acylation must likewise distinguish

$$2'\text{-O acylation} \tag{1084}$$

from possible 3'-O, 5'-O, N-acylated, phosphorylated, or other products.

Define the regioisomer label

$$\zeta_{\text{Ado}} \in \{2'O, 3'O, 5'O, N, \text{other}\}. \tag{1085}$$

The target certificate requires

$$\boxed{\zeta_{\text{Ado}} = 2'O}. \tag{1086}$$

G.16 Experimental stereochemical certification

The product stereochemical certificate requires assignment of

$$\chi(c_{\alpha}). \tag{1087}$$

If both enantiomeric product classes are experimentally measurable, let

$$x_{\star}, \quad x_{\text{opp}} \tag{1088}$$

be their normalized fractions with

$$x_{\star} + x_{\text{opp}} = 1. \quad (1089)$$

Define

$$ee = |x_{\star} - x_{\text{opp}}|. \quad (1090)$$

A practical realization criterion may require

$$x_{\star} \geq x_{\min} \quad (1091)$$

or

$$ee \geq ee_{\min}, \quad (1092)$$

for prospectively declared thresholds.

Such an experimental criterion establishes preferential stereochemical formation at the selected resolution. It is conceptually distinct from the mathematical condition in which the opposite cage branch is empty.

G.17 Cross-validation of computation and experiment

Let

$$D_j^{\text{comp}} \quad (1093)$$

and

$$D_j^{\text{exp}} \quad (1094)$$

be computational and experimental evidence for the same realization hypothesis.

Define a prospectively specified compatibility relation

$$D_j^{\text{comp}} \sim_j D_j^{\text{exp}}. \quad (1095)$$

Compatibility may require, as appropriate: agreement of product connectivity, agreement of isotope provenance, agreement of stereochemical sign, or structural consistency between computed and measured cage observables.

Definition G.2 (Cross-validated hypothesis). A realization hypothesis H_j is *cross validated* when both computational and experimental certificates exist and satisfy the declared relation

$$D_j^{\text{comp}} \sim_j D_j^{\text{exp}}. \quad (1096)$$

G.18 Certification of local transformation invariance

For every $\Lambda \in \mathcal{L}$, family-level certification requires more than one optimized endpoint geometry.

First, candidate transported lifts

$$\tilde{\gamma}_i^{\Lambda} \quad (1097)$$

must be constructed for every transported canonical generator.

Second, compute the augmented hard-constraint deviation

$$\Delta_{\mathcal{F}}^{\Lambda}. \quad (1098)$$

The primary invariance criterion is

$$\Delta_{\mathcal{F}}^{\Lambda} < m_{\min}. \quad (1099)$$

If the cross-realization modulus of continuity of Appendix D.4 has been established, the coordinate-space criterion

$$\varepsilon_{\Lambda} < \varepsilon_0 \quad (1100)$$

may be used as a sufficient condition.

It does not replace the requirement that a candidate transported path exist.

For stereochemical transport, additionally require

$$\sup_t \left| \tilde{\zeta}_{\chi}(t) - \zeta_{\chi}(t) \right| < \delta_{\chi}. \quad (1101)$$

G.19 Certification of dual-cipher and anchor variants

For the $C5 \rightarrow C6$ dual-cipher realization, define an independent gate vector

$$\mathcal{G}^{5 \rightarrow 6} = (G_0^{5 \rightarrow 6}, \dots, G_7^{5 \rightarrow 6}). \quad (1102)$$

Graph-level transport does not identify

$$G_j^{6 \rightarrow 5} \quad (1103)$$

with

$$G_j^{5 \rightarrow 6}. \quad (1104)$$

In particular, the realization should report independently:

$$\Delta \Delta G_{\chi}^{\ddagger}(6 \rightarrow 5) \quad (1105)$$

and

$$\Delta \Delta G_{\chi}^{\ddagger}(5 \rightarrow 6), \quad (1106)$$

as well as the corresponding cage observables.

For adenine-anchor comparison, define independent certificate packages for

$$\eta_A = C2 \quad (1107)$$

and

$$\eta_A = N6. \quad (1108)$$

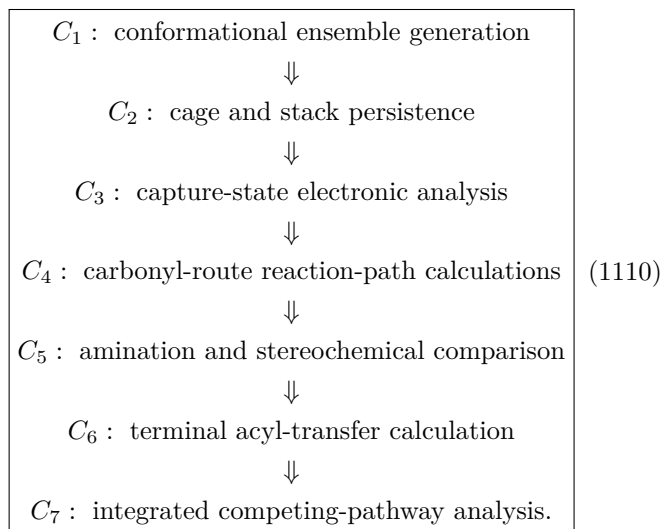
The comparison should report, where applicable,

$$\Delta d_{\pi}, \quad \Delta s_{\pi}, \quad \Delta \Theta_{\pi}, \quad \Delta d_{\text{cap}}, \quad \Delta d_{\text{acyl}}, \quad \Delta \Delta G_{\chi}^{\ddagger}. \quad (1109)$$

The purpose is to determine whether the alternative realization preserves the certified theorem hypotheses, not to presume equivalence with the reference anchor.

G.20 Prospective computational workflow

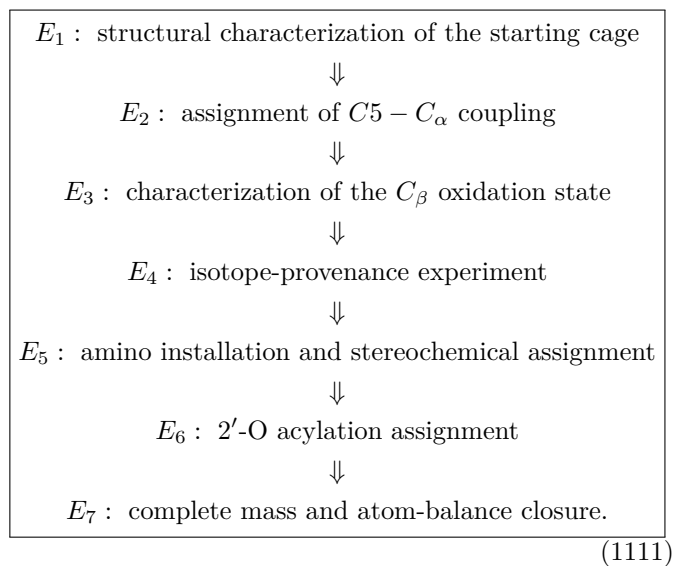
A practical reference workflow may be organized as



The methods and acceptance criteria associated with each stage should be declared prospectively rather than selected solely after the desired outcome is observed.

G.21 Prospective experimental workflow

A corresponding experimental program may be organized as



Direct observation of every formal intermediate is not mathematically required when other evidence can discriminate the relevant reaction words or certify the required theorem hypotheses.

G.22 Certification matrix

For implementation, define a descriptive evidence matrix

$$M_{\text{cert}} = (m_{ij}), \quad (1112)$$

where rows index realization hypotheses and columns index evidence classes.

For example,

	geom.	electr.	kinetic	isotope	product
H_{cap}	m_{11}	m_{12}	m_{13}	m_{14}	m_{15}
H_{carb}	m_{21}	m_{22}	m_{23}	m_{24}	m_{25}
H_{am}	m_{31}	m_{32}	m_{33}	m_{34}	m_{35}
H_{tr}	m_{41}	m_{42}	m_{43}	m_{44}	m_{45}

(1113)

Use

$$m_{ij} \in \{1, 0, \emptyset\}, \quad (1114)$$

where 1 denotes evidence satisfying the declared criterion, 0 denotes disqualifying evidence, and $\emptyset$ means that the evidence class has not been evaluated.

The matrix is descriptive. It does not replace the theorem's logical certificate-support sets.

G.23 Methodological cautions

A visually plausible molecular drawing does not by itself establish

$$\mathcal{K}(S) \neq \emptyset \quad (1115)$$

for a populated molecular ensemble, nor does it establish

$$\text{Lift}_{\mathcal{C}}(p; S, T) \neq \emptyset. \quad (1116)$$

Likewise, a favorable endpoint free-energy difference

$$\Delta G < 0 \quad (1117)$$

does not establish an experimentally accessible barrier

$$\Delta G^\ddagger. \quad (1118)$$

A favorable transition-state energy also does not establish that the required cage geometry has appreciable population.

Accordingly, a full realization certificate may require both

$$P_{\text{cage}} \quad (1119)$$

and an appropriate kinetic or electronic-path observable.

For computational prioritization one may define a heuristic score

$$Q(f) = Q_{\text{geom}} Q_{\text{electronic}} Q_{\text{kinetic}} Q_{\text{stereo}} Q_{\text{transfer}}. \quad (1120)$$

Such a quantity may be useful for selecting realizations for further study, but it is not substituted for the individual logical hypotheses of the existence theorem.

G.24 Prospective falsification criteria

A selected realization route is rejected when a required certificate receives status F.

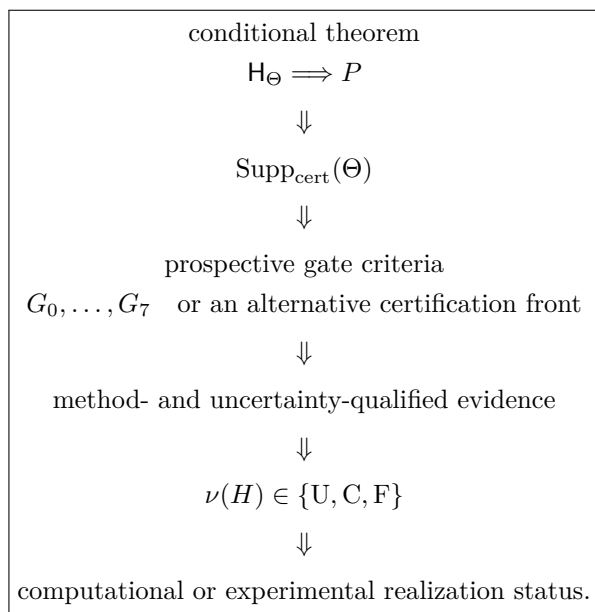
Examples include:

1. absence of a cage population satisfying the required $C5 - C_\alpha$ capture geometry;
2. absence of an admissible electronic route for the selected capture realization;
3. unavoidable destruction of a protected chrysene carbon-framework relation;
4. failure to form the required C_β carbonyl while retaining the necessary leaving-group architecture;
5. failure to install n_α at c_α ;
6. a stereochemical result incompatible with the theorem branch requiring $\chi_\star$;
7. dominant transfer to phosphorus rather than the intended C_β acyl center;
8. terminal acylation inconsistent with 2'-O attachment; or
9. isotope provenance inconsistent with the atom map asserted by a mechanism-specific reaction word.

Falsification of one route removes that route from the applicable certification front. It does not establish failure of target reachability when an independent certified route remains.

G.25 Integrated certification summary

The complete certification program can be summarized as



(1121)

This appendix supplies the implementation details. The mathematical theorem itself remains the conditional implication proved in Section 9.

H Literature Review: From Encoded Chrysene Registries to Cage-Constrained Chemical Processing

The present reaction theory is downstream of a sequence of papers that progressively recast the chrysene architecture from a fixed molecular reference object into an information-bearing stacked system with registry structure, finite classification, and constrained production rules. The purpose of this appendix is to locate the current cage-constrained reachability problem within that development. The prior papers are used here as literature context rather than as premises that establish the chemical feasibility of the reaction generators in Sections 8–11.

H.1 From a molecular anchor to a mathematically controlled realization program

The editorial survey of the Chrysene Formalism described the program as a candidate mathematical and biogenetic framework built around an externally fixed molecular reference structure, while explicitly separating established mathematical structure from unproved realization and identification hypotheses [Sch26a]. The revised twelve-axiom formulation then made that separation formal: the canonical chrysene carbon framework, the tensorial $\mathbb{Z}^3$ network, the primary–dual locant system, the noncommutative sequence algebra, and the spectral layer were reconstructed as distinct mathematical objects, with downstream physical response and admissibility left to separately stated realization hypotheses [?].

This distinction is directly relevant to the present paper. The chemical reachability theory developed here does not infer a reaction mechanism from the existence of the chrysene formalism. Instead, it adds a new realization layer in which persistent atoms, local chemical rewrites, cage geometry, stereochemical selection, and certification are typed explicitly. In this sense, the present work continues the same methodological principle:

$$\boxed{\text{fixed structural information} + \text{explicit realization rules} \implies \text{derived}} \quad (1122)$$

H.2 The encoded stack as an information-bearing object

A second stage of the literature moved from the isolated chrysene node to a stacked and frame-indexed representation. *The Encoded Stack* introduced a base-four structure on the $\mathbb{Z}^3$ -fibrated chrysene network and treated the

stack, its marker data, and its frame structure as objects that carry information [Sch26b]. In the subsequent concordance literature, the marker was retained explicitly as information-bearing, while the frame action, registry coordinates, and multiple descriptions of one stack were kept mathematically separate from physical claims about a realized biochemical code.

This shift is important for the present reaction problem. Once a stack or cluster is treated as an information-bearing object, a physical realization must do more than preserve molecular identity. A local transformation that is intended to act on the encoded object must also preserve the distinctions on which the encoded state depends. That observation motivates the use here of persistent atom maps, protected graph invariants, completed reaction support, and stereochemically typed target classes. The informational literature does not itself prove that a particular reaction performs such processing; rather, it identifies the structural information whose chemical processing must be specified precisely if the proposed realization is to preserve it.

H.3 Registry classes, finite capacity, and the need for precise local processing

The Twenty Registry Classes of a Chrysene Stack classified the frame orbits of a six-unit chrysene stack and obtained twenty registry classes [Sch26e]. The later capacity analysis sharpened the interpretation of those classes. It established, under its stated hypotheses, that a frame class can be treated as one cluster viewed under the available frame conventions, derived an upper bound on the number of distinguishable cluster products, and showed that the bound is twenty for the three-vessel case [Sch26f]. The same analysis separated the capacity bound from the stronger assertion that all classes are chemically realized as distinct products.

That paper also constrained the information available to a production rule. In its formal construction, the production operator is a function of the registry-class data—five binary agreements read modulo end-to-end reversal—rather than of arbitrary absolute orientation or unrestricted external labels [Sch26f]. The result therefore treats the cluster not merely as a spatial assembly but as a finite informational quantity whose admissible output depends on a specific invariant description.

Taken together, the encoded-stack, registry-class, and capacity papers motivate a stronger chemical question:

if the cluster carries distinguishable registry information, what local molecular transformation can process that information without destroying the structural distinctions on which it depends?

(1123)

The present paper addresses one part of that question by replacing an informal chemical arrow with a typed, atom-map-preserving, cage-constrained path. The objective is not to identify the registry classes with the products of the present reaction. It is to supply a mathematical language in which a chemically localized transformation can be checked for conservation, geometric accessibility, stereochemical discrimination, and transport across related realizations.

H.4 Seeded assignments and decision rules

The later registry papers further refine the distinction between information stored in a cluster and information used by a production or reading rule. *Seeded Assignments on the Chrysene Registry* organizes the problem around transversality, third-position refinement, and the mitochondrial code as a proposed normal form [Sch26c]. *Sufficient and Ancillary Reductions of a Chrysene Cluster* continues that program by separating sufficient from ancillary reductions and by treating transverse seeding as a decision rule [Sch26d].

For the purposes of the present article, the important conceptual continuity is that these works make the *rule by which information is selected or reduced* an explicit object of analysis. A registry state does not determine a product merely by existing; a specified selection, seeding, or production rule is required. The current chemical reachability construction adopts the same discipline at the molecular level. The local reaction grammar

$$\mathcal{P} = \{p_\gamma\}_{\gamma \in \Gamma} \quad (1124)$$

is declared explicitly, its complete pattern support is tracked, and its generators must satisfy chemical, geometric, and stereochemical conditions before they are admitted to **Reach_C**.

Accordingly, the registry literature and the present paper address complementary levels:

$$\begin{array}{ll} \text{registry/cluster literature:} & \text{which invariant information and} \\ \text{present reachability theory:} & \text{which atom-resolved local transformation} \end{array} \quad (1125)$$

H.5 Patent architecture and the molecular realization layer

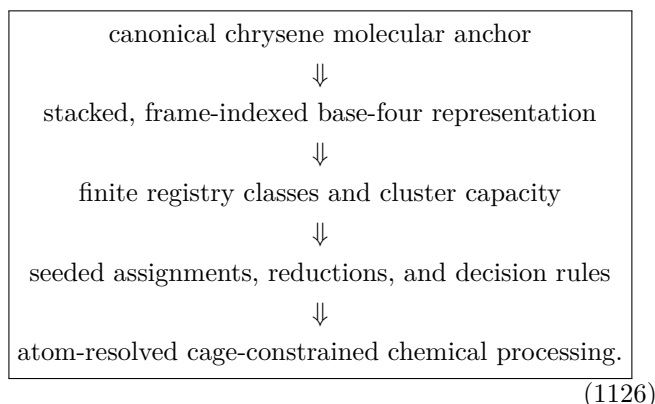
The molecular-development program is also connected to the disclosed architecture of U.S. Patent 12,473,247 B2, *Encoded Design Integrated Synthesis of Nucleic Acids, and Phospholipids, and Related Pharmaceutical Products* [?].

The patent is used in the present literature chain as a documentary source for the molecular realization program: nucleic-acid-linked, phosphate-bearing, and encoded synthetic architectures motivate the class of molecular objects on which the formalism operates.

Patent disclosure and mathematical reachability have different logical roles. The former supplies a disclosed molecular architecture; the latter asks whether a fully specified initial molecular state admits a finite path to a target state under explicit reaction and cage hypotheses. The distinction is the same one enforced throughout this article by Convention 2.2.

H.6 Position of the present work

The prior literature therefore supplies a progression of mathematical questions:



The first four stages concern the structural and informational organization of the chrysene system and the rules by which that information may be classified or reduced [Sch26a, ?, Sch26b, Sch26e, Sch26f, Sch26c, Sch26d]. The present work asks a different but complementary question: whether a specific local chemical transformation can be represented as a finite, atom-balanced, cage-liftable path with a controlled target stereochemistry and with locality sufficient to transport that path across a declared realization family.

In that sense, the principal contribution of the current article is to supply a chemical-processing layer beneath the information-theoretic interpretations of the earlier stack and cluster papers. The result is not an identification of registry information with one unique reaction mechanism. It is a framework in which the physical processing of a declared molecular state can be stated as a falsifiable sequence of chemical, geometric, stereochemical, and certification conditions.

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