

ORTHOGONAL REVIEW RECORD

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

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Review scope

This file is the review record of Article 54. The controlling object is the compiled 94-page manuscript. Omitted source files, intended sections, and unresolved references are not assumed to exist elsewhere. There is no author-reply section.

Scope of Review

The strongest contribution is the separation of graph connectivity, chemical admissibility, cage geometry, and kinetic realization, followed by a categorical treatment in which chemically

admissible local rewrites are refined by nonempty geometric lift spaces. The compiled PDF does not contain the central existence theorem the abstract, introduction, discussion, and conclusion treat as the principal result.

Compiled disposition

Major revision. Invite resubmission after structural repair. Score 73/100. Estimated potential after structural and technical repair: 88–92/100. The core reaction-category architecture is coherent enough to justify revision rather than rejection. Re-review after repair for non-circularity of the main theorem, the repaired perturbative transport result, global conservation bookkeeping, and consistency between theorem scope and the physical certification language.

Required before resubmission

Blocking. Delete the duplicated constructive Section 9 and insert the main existence-theorem section before the alternative-realization section. Rebuild cross-references with labels. Resolve every $[?, ?]$ and add a bibliography. Either rename the perturbative theorem as admissibility persistence for a pre-existing nearby candidate lift, or add a continuous transport map that produces the lift. Restrict the compactness lemma to the projected cage-support space, or bound every coordinate in V .

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1 Score

Category	Score	Assessment
Problem formulation and scope	9/10	Clear question; careful separation of levels
Definitions and type discipline	8/10	Strong; state-space and stereochemical typing to sharpen
Graph rewriting and categorical construction	8/10	Coherent free category; DPO category underspecified
Cage geometry and topology	6/10	Compactness and perturbative persistence need correction
Proof validity and non-circularity	6/10	Central theorem section missing; persistence weaker than worded
Atom, charge, and reaction bookkeeping	8/10	Atom identity is a strength; charge and electron balance implicit
Stereochemical formalization	8/10	Face/CIP separation careful; physical stereospecificity conditional
Locality and substitution invariance	7/10	Graph-level result strong; cage-level transport unclear
Physical-realization boundary and falsifiability	9/10	Certification hierarchy appropriately conditional
Manuscript integrity and editorial readiness	4/10	Duplicate section, missing theorem, unresolved references, no bibliography
Overall	73/100	Major revision

2 What holds

Strengths

The manuscript is more than a speculative mechanism written in mathematical notation. At its best it is a formal language for asking when a proposed local reaction architecture can be represented as a finite path in a constrained reaction category, and how that path behaves under changes of remote molecular context.

Graph-theoretic reachability is not identified with physical feasibility. The cage restricts an admissible state space rather than creating a chemically forbidden transformation. Persistent atom identity, the element map, atom-map-preserving paths, explicit o_x and n_α labels, and terminal coproduct classes are a strength. Appendix A makes carbonyl-oxygen and 2'-oxygen provenance explicit. The graph-level context-extension theorem is one of the strongest results: reaction inert does not imply physically irrelevant. The oriented local frame and the separate map $\kappa_\alpha : \{-1, +1\} \rightarrow \{R, S\}$ postpone L/D assignment until the realized product and CIP ordering are specified. The free category retains distinct reaction words, so reachability does not require a unique mechanism. The gates $G_0, \dots, G_7$ give a falsification interface. A failed mechanism does not invalidate target reachability if another certified path remains.

3 Major issues

Assembly

Section 8 already contains the constructive $C6 \rightarrow C5$ witness. Section 9 repeats that section instead of presenting the promised existence theorem. The introduction, Sections 10 and 11, the discussion, and the conclusion refer to a theorem that is not in the compiled PDF.

Retain one constructive-witness section. Replace the duplicate Section 9 with a theorem that, for each substitution context Λ , there exists a terminal state in the starred target class with a nonempty hom-set in the $6 \rightarrow 5$ reachability category, under a minimal enumerated hypothesis package. The proof should cite the witness-composition theorem and the substitution-invariance theorem, not reproduce the reaction sequence.

The duplicate has left stale numbers: Hypothesis 9.5, Hypothesis 9.7, Proposition 9.11, Theorem 9.16, and Hypothesis 9.17 are cited forward while located in Section 8. Use labels only. After the replacement, audit every cross-reference.

Citations render as [?, ?], including the patent family and the inherited formalism. Appendix F is unresolved. A paper whose architecture is inherited cannot be published without source attribution. The bibliography should include the controlling Chrysene papers, the concordance and directional papers, the two patents as motivating sources only, a standard reference for double-pushout rewriting, and chemistry references for the named interpretations if they remain. Patents are not proof. The bibliography should say so.

Two mathematical corrections

The perturbative theorem assumes a corresponding candidate lift as part of the definition of an ε -small perturbation. It proves persistence of admissibility for a pre-existing nearby path, not existence of a nearby path from small perturbation alone. The compactness lemma bounds the finite cage support $C(S)$ and concludes compactness of the full gauge-fixed set.

Two acceptable repairs of the perturbation theorem. Rename it as persistence of admissibility for uniformly close candidate lifts, and state that it does not establish existence of the lift. Or introduce a continuous transport map from the reference lift space to the perturbed configuration space, and then use the positive-margin argument. The same qualification belongs in the substitution-invariance theorem and the stereochemical-persistence corollary.

For compactness, either state the lemma on the projected cage-support space, or bound every coordinate in V and close the noncollision condition by a positive minimum distance. The extreme-value corollary follows on the corrected domain.

Global charge and redox balance should be invariants, not an open-ended clause inside Chem. Define a total charge-resource quantity and require it constant along a path. An analogous electron balance applies when electrons are explicit resources.

The locality theorem uses a support U_6 . The canonical word later adds o_x , n_α , explicit hydrogens, and reagent-side atoms. Define one canonical support U_{rxn} once, and state locality relative to it.

An elementary cage transition is a quadruple plus a nonempty lift space. A particular geometric

lift is not morphism data. A hom-set of size at least two counts distinct reaction words, not necessarily distinct physical trajectories. Call this grammar-level or reaction-word nonuniqueness unless morphisms are enriched by selected lift classes.

4 Mathematical audit

The atom-universe construction is sound. Replace the single stereochemical map on vertices and edges by separately typed maps, so that R is not assigned to a double bond or E to a tetrahedral atom. State whether the reference embedding ι lies in $\mathcal{K}(S)$ or is only a coordinate set. Split Chem into valence, element balance, charge balance, protected invariant, and a realization-specific remainder, so that theorems do not become tautological. Appendix B treats bond-order change as deletion of one labeled edge and insertion of another. Name the category: finite typed simple graphs with edge labels, or another specified adhesive category. The free-category construction is correct once the quiver is fixed. Keep the full free category distinct from the thin reachability category. The graph-level context-extension argument is a genuine theorem under strong support and inertness hypotheses. A geometric lift is a continuous admissibility homotopy, not a dynamical trajectory, until electronic certification. The stereochemical implication is valid as a conditional statement and does not establish that amino installation is stereospecific. Two distinct words with the same source and target are distinct morphisms. The physical reading stays qualified.

5 Chemistry

The following remain realization hypotheses: cleavage of the $C6-O-C_\alpha$ linkage with productive $C5-C_\alpha$ capture; dehydrogenation of the saturated $C_\alpha-C_\beta$ segment; selective oxygen addition; rearrangement to $C_\beta=O$ while retaining the $C_\beta-O_\beta-P$ linkage; amino installation at C_α ; stereochemical discrimination in the cage; preferential 2'-O acyl transfer over phosphoryl transfer, hydrolysis, or other ribose regioisomers. The isotope prediction $o_x \mapsto o_{\text{carbonyl}}$ distinguishes some competing mechanisms. Where the object is an isolated nucleoside, write ribose or adenosine 2'-OH, not RNA 2'-OH. If the product is called L-configured, state the convention. L is not equated with S .

6 Editorial

Every "Section ???" and $[?, ?]$ must be eliminated. Disclaimers that geometric accessibility does not prove kinetics, and that the canonical witness is not a unique mechanism, are correct and too often repeated. After the duplicate is removed, the discussion and conclusion can carry most of them. At 94 pages the paper is long for an article. Move certification matrices to an appendix, shorten repeated scope passages, consolidate notation tables, and leave full DPO edge lists in the appendices. Long arrays are crowded in two columns. Use a full-width environment for the longest diagrams.

Revision sequence

- R1.** Delete the duplicated constructive Section 9 and insert the main existence-theorem section.
- R2.** Rebuild cross-references with labels. Remove hard-coded theorem numbers from prose.

- R3.** Resolve bibliography keys and add a references section.
- R4.** Restate the main theorem in minimal form: connectivity existence, stereochemical existence, and substitution-family transport, separately.
- R5.** Correct the perturbation theorem, by weaker wording or by a continuous transport construction.
- R6.** Correct the compactness lemma.
- R7.** Define global charge and redox invariants.
- R8.** Unify the reaction support as U_{rxn} .
- R9.** Call hom-set multiplicity grammar-level unless lift classes are morphism data.
- R10.** State whether $\iota \in \mathcal{K}(S)$.
- R11.** Use separate atom and bond stereochemical maps.
- R12.** Do not write $\text{Hom}(S, \mathfrak{T}_\star)$ as though the class were an object. Existentially quantify a terminal state, or use the defined coproduct.
- R13.** Add standard literature for graph rewriting, categorical conventions, and the chemical precedents in the certification discussion.
- R14.** Audit dependencies after renumbering.

Suggested theorem schema

Fix $\Lambda \in \{\{6, 12\}, \{3, 6, 12\}, \{3, 6, 9, 12\}\}$. Assume the initial state is chemically and cage admissible; the six canonical local rules have balanced chemical realizations; each rule admits a cage-compatible geometric lift; sources and targets compose in the stated order; the terminal state satisfies the protected-invariant and coproduct conditions. Then there is a connectivity terminal state with nonempty hom-set from the initial state. If, in addition, amino installation is stereospecific and the admissible attack set satisfies the strong selection condition, the terminal state can be chosen in the starred class. If the reference path satisfies the corrected local-transport hypotheses, the same conclusion holds for every Λ in the family. Stereochemistry and substitution invariance are not part of the minimal connectivity theorem.

Decision

Major revision. Invite resubmission after structural repair. The issues do not require abandonment of the program.

References

- [Sch26] Controlling Chrysene Formalism sources, cited in the compiled manuscript as unresolved keys. To be supplied in the repaired bibliography. Patents used only as motivating realization sources.

Revision history

Version	Date	Notes
v1.0	2026-10-07	Review record published with Article 54.

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