ANNALS OF THE CHRYSENE FORMALISM

ORTHOGONAL REVIEW RECORD | VOL. 1, NO. 4 | ISSN 3144-2021 | NOVEMBER 2026

ORTHOGONAL REVIEW RECORD

Emergent Assembly Chirality and Flip Kinematics: Euclidean Stabilizers of the Frame Classes, Enantiotopic Faces of the C_{2h} Core, and Initiator Capping of the Interior Lattice

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Annals of the Chrysene Formalism
Schaper Systems Press

Paper ID:	ACF-1.4-091
Issue:	Volume 1, Number 4, November 2026
ISSN:	3144-2021
Review architecture:	Historical report; mathematical validity (M); concordance (C); chemistry and domain admissibility (H); revision response
Record date:	5 November 2026
Document version:	Publication-package review v1.0
Editorial status:	Prepared for author review; this record does not certify editorial acceptance or publication

Declared review status

This is an AI-assisted simulated review record, not independently appointed human peer review. Separate mathematical and chemistry review passes informed the manuscript revision; concordance checks compare the statement of results, the evidence supporting them and the companion documents. The revision responses describe changes prepared for the author's consideration, not unprovided statements attributed to the author.

Scope of Review

The controlling source is the supplied Article 91 `main.tex`. The earlier `referee_report_a91.tex` and `verify_a91.py` are supporting records, not substitutes for checking the manuscript. Exact combinatorial identities, geometric implications under realization assumptions, reduced interaction models and compound-specific experimental assertions are evaluated separately.

Combined recommendation

Retain the core kinematic and combinatorial program after substantive, scope-preserving revisions. Exact frame counts and locked-sign energy identities survive. The Euclidean interpretation needs explicit realization premises, the primary geometry requires correction, and thermal blindness requires a one-partner-invariant pair measure.

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1 Source record and historical review

The source files are preserved separately from the revised release. The original report is retained unaltered as `provenance/Article91_Prior_Referee_Source.tex`. It carries provisional Volume 1, Number 5, October 2026 metadata and a verdict of "Accept (All Revisions Verified & Incorporated in Step 4)." That sentence is historical evidence of the supplied report's conclusion; it is not the disposition of the present review.

Supplied manuscript SHA-256

`b2fb431eb9c6c98e8a28fbace528284715`

`2608fefaba1bffdce9801999bfe111`

Supplied referee source SHA-256

`df4aceb848954874e64f1a7e8bae623466`

`4fdad0125b0e9b605a6e505d582b2d`

1.1 Substance of the earlier review

The prior report endorsed four conclusions: a rigid-motion classification of the core, a palindrome criterion for assembly achirality, universal chirality after initiator capping, and a sign-conformation contact-bias mechanism. It also recorded five repair groups:

1. Missing imported numeric macros and a table alignment error.
2. Extension of the planar-reflection test from the finite tiling group to all of $O(2)$ using distinct inertia eigenvalues and tests of the two principal-axis reflections.
3. Separation of species-palindromic columns from alternating D, T columns under reversal.
4. Both x-boundary orientations of the initiator in the $3 \times 3 \times 6$ box.
5. Extension of the locked-sign energy formula to mixed sign patterns on T.

These topics remain relevant. The new review does not adopt the prior report's blanket verification claim: a finite check of reversal orbits does not establish that every such orbit is realized by the claimed Euclidean molecular geometry, and the original thermal argument does not follow from equal weights on simultaneously transformed conformers.

2 Review architecture and retained results

> *M* — **Mathematical validity**
>
> Check the exact core isometries, the relation between word actions and physical symmetries, the orbit count, the domain of the probability statements, the capping argument and the partition-sum proof. Preserve valid finite identities while repairing missing premises and false implications.

C — Concordance

Check agreement among abstract, theorem statements, proofs, tables, hypothesis register, numerical examples, verification code, formal certificates and historical review. The same conditional result must not become unconditional in a summary or graphical abstract.

H — Chemistry and domain admissibility

Check what the finite model implies about stereochemistry, flexible arms, interactions, experimental chirality and resource budgets. Identify the additional molecular evidence required without replacing the mathematical paper with an experimental study.

2.1 Results retained independently of molecular realization

For a binary site word $w = (w_0, \ldots, w_{l-1})$, the adjacent-difference field

$$\mathrm{agr}(w)_i = w_i + w_{i+1} \pmod 2$$

is invariant under global complement and commutes with reversal. Each field has precisely two site lifts. Writing $n = l - 1$, the number of reversal-fixed fields and the number of nontrivial reversal pairs are

$$P_n = 2^{\lceil n/2 \rceil}, \qquad Q_n = \frac{2^n - P_n}{2}.$$

At $l = 6$, there are eight fixed fields and twelve two-element reversal orbits, accounting for all 32 fields and twenty frame classes. These are exact finite combinatorial counts. Their interpretation as molecular achirality classes and enantiomeric pairs is an additional geometric statement.

For the specified locked sign model, each anti orbit contributes four units of the coupling constant to the difference of contact energies:

$$E_1 - E_0 = 4 n_{\mathrm{anti}} \epsilon_{\mathrm{syn}}.$$

This identity is preserved as an exact consequence of the stated reduced Hamiltonian. It does not determine the coupling constant for a synthesized compound.

3 Mathematical review and revision response

M1 Separate frame combinatorics from Euclidean realization

Original location: `def:stack_euclid`, `lem:equivariance`, `thm:emergent_chirality`. The original H_{twist} says that assembly isometries act through the frame group. This does not establish the converse: a word operation preserving the field need not be implemented by an isometry of the complete assembly. Nor does it identify all determinant signs, exclude residual symmetries, or ensure that the orientation words are geometrically distinguishable.

Recommendation. State a faithful decorated-realization hypothesis that specifies the admissible layer actions, proper superposability, reflection/reversal correspondence and completeness of the

symmetry classification. Prove the palindrome criterion under those premises. Identify those premises as molecular realization requirements rather than conclusions of the orbit enumeration.

Revision response. The revision separates the unconditional finite frame identities from a conditional geometric interpretation under an explicit realization hypothesis. The converse direction of the achirality criterion is justified only within that declared realization class.

M2 Repair the thermal averaging theorem

Original location: `thm:conformations`(c), its proof and verification block Z7. Let J be the sign permutation induced by $C_2(z)$. For two arm configurations x, y, the reduced interaction is

$$E_\eta(x,y) = -\epsilon \sum_{a\in S} x(a)(J^\eta y)(a).$$

The map $(x,y) \mapsto (x, Jy)$ exchanges E_0 and E_1. The simultaneous map $(x,y) \mapsto (Jx, Jy)$ generally does not. In particular, a correlated ensemble supported on (x,x) and (Jx,Jx) can have equal weights on that pair while retaining the same nonzero energy difference at both configurations.

Recommendation. For the unnormalized pair measure ν, require

$$\nu(x,y) = \nu(x,Jy)$$

or another explicitly stated measure-preserving energy-exchanging involution. Then the substitution $y \mapsto Jy$ yields

$$Z_1 = \sum_{x,y} \nu(x,y) e^{-\beta E_1(x,y)} = \sum_{x,y} \nu(x,y) e^{-\beta E_0(x,y)} = Z_0.$$

Independent marginals with a J-invariant second marginal are one sufficient case. A correlated diagonal ensemble is a necessary negative test.

Revision response. The revised theorem uses the pair-measure condition and an explicit partition-sum proof. The verification suite must exercise both the invariant ensemble and a correlated counterexample; equal marginal weights alone are no longer asserted to suffice.

M3 Correct the primary geometry and covariance data

Original location: `lem:no_refl`, equation for the inertia tensor and verification block Z1. The original printed covariance matrix and its claimed eigenvalues are inconsistent with the supplied 18 carbon coordinates. The centered covariance computed from those primary coordinates is

$$M = \begin{pmatrix} 177/8 & -91\sqrt{3}/8 \\ -91\sqrt{3}/8 & 507/8 \end{pmatrix}, \qquad \lambda_\pm = \frac{171 \pm \sqrt{13017}}{4}.$$

The source's four-cell polyhex also fails its own first stabilizer assertion. A consistent four-cell representation reconstructed from the carbon hexagon centers is

$$\mathcal{S}_4 = \{(0,0), (0,1), (1,-2), (1,-1)\}.$$

Recommendation. Recompute every geometric invariant from the actual coordinates rather than preserving printed constants. Verify central symmetry, the D_6 stabilizer, the exact covariance and

the continuum reflection exclusion in one consistent representation. The correction to the eigenvalues of the *original erroneous matrix* is not a repair of the primary-data mismatch.

Revision response. The replacement verifier uses the primary carbon coordinates and derives the covariance and consistent polyhex. The manuscript's geometric certificate is updated accordingly. The absence of a continuous planar reflection remains a statement requiring its exact argument, not merely a finite tiling-group search.

M4 Replace the overstated inherited verification record

Original location: verification appendix Z1–Z7 and historical referee report. The supplied `verify_a91.py`, run normally, fails its first stabilizer assertion, `s4_rot_stabilizer == [0,3]`. This directly contradicts the inherited report's blanket claim that all verification blocks had passed. Further inspection found that the original enumeration ended at length 12 rather than the claimed 14; it did not test principal-axis reflections, capped-stack stabilizers or annealed cancellation; and several emitted quantities were literal constants. Assertions also disappear under Python's optimization flag.

Recommendation. Replace those checks by explicit failures that remain active in optimized execution, derive claimed constants, test the revised thermal theorem and its counterexample, and give every block an honest coverage statement. Finite enumeration at specified lengths must not be presented as the proof of an arbitrary-length theorem. The Lean companion must distinguish actual compiled certificates from analytic or molecular assumptions.

Revision response. The revised package includes a replacement verifier and a new formal companion. The old code and report are preserved as provenance, not treated as a valid execution certificate. The final execution record below supersedes the historical blanket verification statement.

M5 State the range and meaning of the probability claim

Original location: `cor:racemic_endo`. For uniformly sampled fields,

$$P_{\mathrm{nonpal}}(l) = 1 - 2^{-\lfloor (l-1)/2 \rfloor}.$$

At $l = 3$ this is $1/2$; the exact formula, not a qualitative interpretation, controls all boundary cases. Enantiomeric interpretation also requires the faithful realization and the appropriate species symmetry. For an alternating sequence whose reversal is a different ordered chemical sequence, the ensemble must include the mirror chemical sequence to discuss racemic pairing within a common ensemble.

Revision response. The revised source distinguishes combinatorial reversal-pair probabilities from physical enantiomeric excess and states the ensemble and realization premises. Placement specifies the initial prepared class; it does not by itself establish persistence or kinetic stability.

M6 Restrict the capping conclusion to its geometry

Original location: `thm:capped_chirality`, `prop:cap_budget` and synthesis table. An end-specific chemical cap can exclude layer reversal, but the absence of all other improper symmetries must come from a complete geometric symmetry classification. A cap count on a multi-column

lattice is not a proof that the entire lattice has trivial stabilizer: global operations may permute equivalent columns.

Revision response. The revised discussion separates conditional single-column symmetry, local bridge compatibility and the resource count for a larger lattice. A global lattice chirality assertion requires its own fully decorated geometry and symmetry analysis.

M7 Repair status and imported-source correspondence

The original theorem status labels, imported Article 90 title and proposition references must match the current source and the actual logical dependencies. A statement that uses the realization hypothesis is conditional even when its finite combinatorial ingredient is exact. The prior referee's acceptance is a historical claim, not newly verified evidence.

Revision response. The revision uses the approved Article 90 source, corrects metadata and labels, and explicitly separates the source record from current review and verification.

4 Concordance review and revision response

C1 Synchronize the hypothesis boundary across the package

The abstract, introduction, non-implications proposition, synthesis table, precedence rulings and conclusion must all distinguish the exact frame count from its conditional Euclidean interpretation. The historical description "discharge unconditionally" must not survive as a claim about a decorated physical stack.

Revision response. Summary language is revised to agree with the explicit realization assumptions. The historical report remains in provenance and is superseded where it overstates the conclusion.

C2 Distinguish word labels from physical orientation

A bare C_2-symmetric core is unchanged as an unlabelled carbon framework by $C_2(z)$. Consequently, $w = 0$ and $w = 1$ do not automatically represent distinct physical configurations. Arbitrary locant labels cannot manufacture a measurable distinction.

Revision response. The faithful realization uses physical decoration or environmental distinctions where required; the binary word is otherwise treated as a model coordinate. Claims of physical chirality are confined accordingly.

C3 Keep the energy model and probability convention consistent

The logistic formula uses a specified contact orientation, a definite $\Delta E = E_1 - E_0$, and $\beta = 1/(k_B T)$. A statement that any nonzero coupling gives a nonzero bias is only valid when $n_{\mathrm{anti}} > 0$. Sign reversal of the coupling changes the favored registry.

Revision response. The model interpretation, mathematical formula and verification examples are kept aligned. Neither the sign nor the magnitude of a compound-specific interaction is inferred from the sign count.

C4 Reconcile imported values and cap-budget claims

The source's flux, efficiency and cap-surplus values are imported model parameters, not experiments carried out for this article. A positive aggregate surplus does not guarantee timely transport, binding, correct orientation or retention of initiators at every desired site.

Revision response. The manuscript describes the arithmetic as conditional stoichiometric sufficiency and distinguishes supply, local placement and global assembly. Imported quantities are not represented as newly measured chemical efficiencies.

C5 Align the supplements, metadata and abstract

The new verification and Lean files must correspond to the revised statements, including tests capable of detecting the incorrect thermal claim. The OJS abstract must be derived from the manuscript abstract, preserving math delimiters while removing typography commands. All documents use Article 91, Volume 1, Number 4 and November 2026.

Revision response. The package carries an explicit coverage ledger and synchronized descriptive metadata. Formal-proof scope is stated separately from mathematical and chemical conclusions. The manuscript, report and supplements are delivered as a coherent publication package.

5 Chemistry review and revision response

H1 Require a faithful molecular realization

A half-turn of a bare C_{2h} core or a fully C_2-symmetric decorated unit returns the same spatial structure. Binary orientation labels alone cannot alter its Euclidean stabilizer. A qualitative appeal to ordinary π stacking does not provide a faithful and complete determinant-graded action of the frame group or prove that layers are geometrically recognizable.

Revision response. The revision retains the exact registry counts and states the added orientation-sensitive decorated-realization premises needed for the physical chirality interpretation. This is a conditional-theorem repair, not a claim of established molecular coordinates.

H2 Separate sign stabilizers from molecular point groups

Equal terminal-height signs do not imply equal arm torsions, lengths or all-atom coordinates. Opposite signs do not establish inversion symmetry of a complete flexible molecule. The terms syn and anti are local shorthand for terminal half-space signs in this model.

Revision response. The $2 + 2$ classification on D and $4 + 4 + 8$ classification on T are retained as exact sign-model stabilizers. An atomistic C_2, C_i or C_1 assignment requires an equivariant coordinate realization.

H3 Correct the thermal ensemble premise

Equal one-partner marginals and invariance under simultaneous transformation do not establish thermal blindness. For D, $x = (+1, -1)$ and $Jx = (-1, +1)$ give $E_0 = -2\epsilon$ and $E_1 = 2\epsilon$ for both

diagonal pairs (x, x) and (Jx, Jx). Their equal mixture retains a bias.

Revision response. The revised theorem uses invariance under the one-partner bijection $(x, y) \mapsto (x, Jy)$ and proves equality by changing the second summation variable. The fixed-conformer Boltzmann bias presumes registry equilibration and the specified degeneracy, not an arbitrary kinetically trapped contact. The correlated example is included as a negative control.

H4 Distinguish core kinematics from reaction pathways

An improper operation is not a continuous rigid rotation. Group classification neither establishes a chemically permitted arm-inversion pathway nor determines its barrier. A physical facial turnover is possible but changes the canonical footprint. The correct achirality criterion is proper superposability with the mirror image, equivalently the existence of an improper stabilizer. Clockwise traversal of locant labels alone is not a stereochemical criterion.

Revision response. The revised core theorem states its footprint-preserving restriction and describes improper inversion as a coordinate symmetry relation. The facial argument uses the absence of a face-exchanging proper stabilizer, with an explicit face-specific marking or complexation interpretation; it does not prescribe a universal mechanism.

H5 Refine nomenclature and ensemble conclusions

The capped family has not been shown to consist entirely of diastereomers, and unassigned d/l labels risk implying optical rotation or a D/L configuration that the model does not provide. A mirror-invariant probability law gives equal ideal populations, not exact zero excess in every finite batch. An achiral cap alone is not proof of homochiral synthesis.

Revision response. The revision uses chiral capped configurations and enantiomeric-pair language within the assumed realization. Ideal one-enantiomer preparation is distinguished from finite sampling and subsequent racemization. Persistent assignment requires interconversion to be slow relative to observation or storage.

H6 Separate cap mass balance from chemical feasibility

The fluxes 20.8 and 19.8 are model mean counts per period. They do not establish transport, capture, selective binding or retention. Six boundary columns admit the local in-layer initiator replacement; all nine require the separately stated terminal-overhang construction. A mean surplus of 19.8 exceeds rather than equals the demands of nine or eighteen caps. The imported efficiency 0.998437 is not a measured synthesis yield.

Revision response. The revision keeps the ideal arithmetic while separating supply, geometry and chemical assembly. Whole-lattice symmetry and double-ended capping require separate analysis; a one-column theorem is not silently extended to either.

H7 Calibrate the effective interaction and timescale

The bilinear sign coupling is phenomenological. Its coefficient has units of energy; temperature is positive; and the probability convention must identify $\eta = 1$. Terminal signs relative to two planes

do not determine actual separations or the sign of intermolecular forces. A contact free-energy difference is not an inversion barrier.

Revision response. The model energy identity remains exact within its assumptions. Molecular calculations or measurements must calibrate coupling, degeneracies, solvent effects and exchange rates. The manuscript distinguishes a proposed interaction model from an atomistically derived potential.

H8 Make experimental closure discriminating

Chirality permits but does not guarantee detectable circular dichroism at every wavelength. Mirror-related enantiopure preparations in an achiral environment should give opposite spectra where nonzero, and an ideal racemate cancels. A null signal alone does not prove an achiral or meso structure.

Revision response. The revised target calls for structural and chemical identification, enantiomer-resolved or chiroptical tests with racemate and achiral controls, aggregation/concentration dependence, and checks for linear-dichroism or scattering artifacts in oriented samples. Barrier calculations require a pathway; variable-temperature NMR requires resolvable exchanging signals. These tests are proposals, not claimed completed experiments.

5.1 Terminology sources

The chemistry review consulted the IUPAC Gold Book entries for chirality, enantiotopic, meso, enantiomeric excess and dichroism, together with the IUPAC stereochemistry recommendations:

- Chirality: `https://doi.org/10.1351/goldbook.C01058`.
- Enantiotopic: `https://doi.org/10.1351/goldbook.E02083`.
- Meso: `https://doi.org/10.1351/goldbook.M03838`.
- Enantiomeric excess: `https://doi.org/10.1351/goldbook.E02070`.
- Dichroism: `https://doi.org/10.1351/goldbook.DT07357`.
- Basic terminology of stereochemistry: `https://doi.org/10.1351/pac199668122193`.

6 Disposition and preservation of the central program

The substantive recommendations are accepted in scope. They preserve the finite frame algebra, its exact orbit counts, the idealized core kinematics and the locked-sign contact identity. They qualify the interpretation of those results and repair the thermal proof. There is no need to replace the paper with a different scientific program or to add unsupported experimental claims.

A demand that the paper establish compound-specific synthesis, a stable atomistic conformer or measured optical activity before presenting a conditional theorem would exceed its mathematical purpose. Such evidence is necessary for the corresponding physical realization claim, not for the finite algebraic identity. Conversely, calling a geometric result conditional cannot rescue a false implication: the realization hypotheses and pair-measure condition must be stated explicitly and used in the proof.

7 Verification record and final package check

The replacement Python verifier passed 108,715 explicit checks in each of normal and optimized execution. Ten deliberate negative controls were rejected. The finite word enumeration covers lengths $2 \leq l \leq 14$; the capped-frame checks cover $2 \leq l \leq 8$. The geometry checks reconstruct the corrected chrysene polyhex and carbon coordinates, derive the covariance, and test the finite reflection reduction. They do not classify all seven four-cell polyhex isomers. All D and T sign states are checked, together with energy exchange and the correlated anti-state counterexample.

The new Lean 4.24 source compiled successfully and its dependency audit checked 38 named theorems. Thirty-six finite certificates use kernel decision and have no axioms in their printed dependency lists. Two general list identities, double complement and adjacent-difference invariance under complement, use only Lean's standard propositional-extensionality axiom (`propext`). The source contains no `sorry`, `admit`, custom axiom or `native_decide`. These certificates do not formalize the full Euclidean molecular realization, arbitrary-length orbit-count theorem or partition-sum theorem. Those remain manuscript arguments with their stated premises.

Independent mathematical and chemistry closure passes confirmed that the substantive recommendations were implemented. The final consistency pass corrected residual summary wording concerning species-symmetric field counts, improper self-isometries and sign-model classification. These checks support the revised conditional result; they do not certify experimental feasibility.

Verification scope

The verification code tests finite symmetries, orbit counts, reduced sign energies, thermal change-of-variables cases and specified resource arithmetic. The Lean companion supplies explicitly listed finite or algebraic certificates. Any use of a native decision procedure, external computation, finite bound or unformalized analytic premise is declared in that companion.

Final recommendation

The revised work is suitable for the author's publication decision as a conditional mathematical model with an explicit experimental-realization boundary. The substantive mathematical, concordance and chemistry recommendations have been incorporated, and the new verification and formal companions provide the scoped execution record stated above. This recommendation is a simulated technical assessment, not an external editorial acceptance.