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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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Abstract

The canonical planar chrysene carbon framework has point group C_{2h} and no reflection symmetry within its plane. We establish that its locant involution is induced by the in-plane half-turn $C_2(z)$; no proper face-exchanging rotation preserves the same carbon footprint. We then separate the finite registry classification from its geometric realization. Under an explicit faithful, reflection-equivariant decorated-realization hypothesis, a species-symmetric stack is achiral precisely when its alignment field is palindromic. At length $l = 6$, the 32 fields comprise 8 achiral fields and 24 chiral fields forming 12 mirror pairs. Uniform endogenous draws are racemic at the ensemble level, whereas ideal placement can select one member of a pair. A unique asymmetric terminal cap removes the candidate nonidentity stabilizers under the stated layer-preservation and realization conditions. The imported matched-source model yields an initiator surplus of 19.8 units per period, exceeding the separate resource demands of 1, 9, or 18 caps; saturated in-layer placement is available only on the compatible boundary columns, while other columns require external overhangs. Finally, a finite arm-sign model partitions the D and T states by stabilizer and gives an explicit orientation bias for fixed, identical anti or mixed states. Thermal restoration of blindness follows from invariance of the joint conformational measure under a single-partner half-turn. A correlated anti-state counterexample shows why symmetric one-unit marginals alone do not suffice. Exact enumeration, new verification code, and finite Lean certificates support the algebraic statements; the geometric and chemical interpretation is stated through explicit realization assumptions.

Keywords: Chrysene Formalism; assembly chirality; Euclidean stabilizer; registry reversal; enantiotopic faces; initiator capping; conformational bias.

1 Introduction

1.1 From combinatorial involution to Euclidean motion

Across Articles 79, 84, and 90 [Sch26g, Sch26e, Sch26f], the reference symmetry of the chrysene core enters the combinatorics of the stack through a single permutation of the primary locants $\Lambda = \{3, 6, 9, 12\}$: the involution ι acting as $3 \leftrightarrow 9, 6 \leftrightarrow 12$ [Sch26a, eqs. (52)–(53), (661)]. In Article 79, ι singles chrysene out among the 7 four-ring polyhexes as the unique C_{2h} skeleton whose continuous arm registrations exclude four-ring competitors at the column [Sch26g, Prop. 4.4, Cor. 8.6]. In Article 84, that same involution proves unit and contact blindness: because $D = \{6, 12\}$ and $T = \{3, 6, 9, 12\}$ satisfy $\iota S = S$ and carry ι-constant arm words ee and $eeee$ in the one-reagent stock, flipping a unit leaves its presented locant-arm pattern invariant, rendering Article 79's registration filter blind to the alignment field $\eta \in \{0, 1\}^{l-1}$ at every $\{D, T\}$-contact [Sch26e, Thms. 7.3–7.4].

What the combinatorial treatment deliberately leaves open is the three-dimensional Euclidean geometry of that flip and of the stacks it generates. Article 40 formulates the symmetry hierarchy of the Chrysene Formalism in $E(3) = O(3) \ltimes \mathbb{R}^3$, distinguishing the canonical carbon-framework point group $\Pi_{\mathfrak{C}}^{\mathrm{core}} \sim_{O(3)} C_{2h}^{\mathrm{std}}$, the embedded carbon-framework stabilizer $\Gamma_{\mathfrak{C}}^{\mathrm{emb}}$, the full labeled node stabilizer $\Gamma_{\mathfrak{C}}$ [Sch26a, eq. (47)], and the Euclidean stabilizer $\Gamma_{\mathfrak{S}} \leq E(3)$ of a stacked assembly [Sch26a, Def. 84]. Because C_{2h}^{std} contains spatial inversion $-I_3$ and horizontal reflection σ_h, both of determinant -1, the isolated chrysene core is achiral [Sch26a, Prop. 2], and Axiom A_6 cautions that "the registry label is not identified with molecular chirality" [Sch26a, eq. (109)].

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Instead, Article 40 poses emergent supramolecular chirality as a deferred theorem target ([Sch26a, Thm. 47]): determining which admissible registry sequences $\{\eta_k\}$ eliminate every improper symmetry ($\det R_g = -1$) from the assembled stabilizer $\Gamma_{\mathfrak{S}}$.

1.2 Four open targets on the geometry of the stack

Four explicit targets in Articles 40 and 84 meet at this point:

(i) *Which rigid motion the flip is ([Sch26e, Rem. 4.7, Target 14.11]).* Article 84 notes two candidate readings for the flip $\eta_k \mapsto \eta_k + 1$: an in-plane reorientation by the non-trivial rotation of C_{2h}, or a turning-over of the molecular plane exchanging its two faces. Both induce ι on Λ, so Article 84's combinatorial theorems hold under either, while leaving the physical identification as Target 14.11.

(ii) *The Emergent Chirality Theorem ([Sch26a, Def. 84, Thm. 47]).* Which of the 2^{l-1} alignment fields (and which of the $N(l)$ frame classes of [Sch26e, Thm. 6.5]) yield a chiral assembly satisfying $\Gamma_{\mathfrak{S}} \cap \{g \in E(3) : \det R_g = -1\} = \emptyset$, and how do the endogenous and placed sources weight the chiral and achiral sectors?

(iii) *A frame carrier on the column and lattice ([Sch26e, Target 14.14]).* Can the trisubstituted initiator $I = \{3, 6, 12\}$ sit at the terminus of a column or on a face of Article 80's $B(3, 3, 6)$ interior lattice [Sch26c] so as to fix the frame and break improper symmetry, and does Article 79's stream ($p_3 = 4.88 \times 10^{-4}$) supply enough initiator units per period?

(iv) *Conformational orientation bias ([Sch26e, Target 14.1]).* When the flexible hydroxyethoxy arms project out of the molecular plane, under what condition do non-centrosymmetric or centrosymmetric arm conformations create a free-energy difference ($\theta \neq 1/2$) between the two alignment states of a D or T contact?

1.3 What is established here, by kind

Recovered. Article 40's polyhex enumeration $\mathcal{P}_4 = \{\mathcal{S}_1, \ldots, \mathcal{S}_7\}$ and symmetry table ([Sch26a, Thm. 51, Prop. 53, Table 1]); its three-level stabilizer hierarchy and achirality proof for C_{2h} ([Sch26a, Axiom A_2, Prop. 2]); its assembly stabilizer and emergent chirality target ([Sch26a, Def. 84, Thm. 47]); Article 79's matched exit distribution and initiator throughput $\Phi_{\min} p_3 = 20.8$ per period ([Sch26g, Cor. 7.4]); Article 80's $B(3, 3, 6)$ heritable minimum [Sch26c]; Article 84's frame-class count $N(l)$, agreement-word quotient Lemma 8.10, and Targets 14.1, 14.11, and 14.14 [Sch26e].

Proved here. The core kinematic result is exact for the displayed canonical coordinates. The word and arm-sign enumerations are finite algebraic results. Their chirality interpretation requires the faithful decorated realization in Definition 4.1; this supplies the sufficient geometric condition that an action constraint alone cannot provide. The cap theorem and material ledger have separate symmetry, placement, and resource premises. The contact-energy calculation is an explicit model, and its annealed conclusion uses a joint-measure invariance condition rather than symmetry of one-unit marginals alone.

2 Conventions, nomenclature, and non-implications

Convention 2.1 (Status labels and documentary marks)**.** Every numbered statement carries one of four labels: **[A]** finite, algebraic, or axiom-free; **[D]** derived under hypotheses named and registered in Appendix A; **[C]** imported from a cited source; **[E]** a molecular or patent reading, entering no proof. Scholia are unlabelled and enter no proof. The filing [Sch25] is cited via Article 65's bundle H_{mat} [Sch26b] as amended by clause (i) of [Sch26g] and clause (j) of [Sch26e]. Derived numerical macros are generated and checked, while imported model inputs are explicitly tagged, by `verify_a91.py` (blocks Z1–Z7, Appendix C).

Notation 2.2 (Euclidean and point-group data)**.** $E(3) = O(3) \ltimes \mathbb{R}^3$ the Euclidean group with elements $g(r) = R_g r + t_g$ ($R_g \in O(3), t_g \in \mathbb{R}^3$); $SE(3) = SO(3) \ltimes \mathbb{R}^3$ the proper subgroup ($\det R_g = +1$); $\hat{\iota}_{\mathrm{px}} : V_{\mathfrak{C}} \to \mathbb{R}^2 \times \{0\} \subset \mathbb{R}^3$ the canonical regular-polyhex embedding of [Sch26a, eq. (43)]; $C_{2h}^{\mathrm{std}} = \{I_3, C_2(z), \sigma_h, -I_3\} \leq O(3)$ where $C_2(z) = \mathrm{diag}(-1, -1, 1)$, $\sigma_h = \mathrm{diag}(1, 1, -1)$, and $-I_3 = \mathrm{diag}(-1, -1, -1)$; $\Gamma_{\mathfrak{S}} \leq E(3)$ the Euclidean stabilizer of a stacked assembly $\mathfrak{S}$ ([Sch26a, Def. 84]); $\mathrm{Fr} = \langle \mathrm{flip}, \mathrm{rev} \rangle$ on $\{0, 1\}^l$ and $\mathrm{rev}_\eta(\eta)_i = \eta_{l-2-i}$ on $\{0, 1\}^{l-1}$.

Proposition 2.3 (Non-implications)**. [A]** *None of the following is asserted:*

(i) No 3D chirality of an isolated planar core from two-sidedness. *Having enantiotopic faces does not make an isolated planar D, I, or T core chiral in $\mathbb{R}^3$; $\sigma_h = \mathrm{diag}(1, 1, -1)$ fixes every point in $z = 0$ with $\det(\sigma_h) = -1$, so isolated planar cores are achiral ([Sch26a, Prop. 2, eq. (109)], [Sch26b, Table 1]).*

(ii) No chirality for palindromic registry fields on homotypic stacks. *A binary registry field does not automatically make a homotypic stack chiral ([Sch26a, Rem. 53]); the $2^{\lceil (l-1)/2 \rceil}$ palindromic fields ($\mathrm{rev}_\eta(\eta) = \eta$) retain an improper Euclidean symmetry and are achiral* achiral registry *stacks (Theorem 4.4).*

(iii) No net enantiomeric excess from an uncapped endogenous draw. *Although* 75.0% *of hexamer alignment fields are chiral, the endogenous source assigns equal probability* $2^{-(l-1)}$ *to* η *and its enantiomer* $\mathrm{rev}_\eta(\eta)$*, yielding a mirror-invariant ideal ensemble law. A finite batch can fluctuate, and an achiral cap alone does not guarantee enantiomeric selection (Corollary 4.5).*

(iv) No contact bias from thermally equilibrated achiral arm fluctuations. *Out-of-plane arm displacements do not shift* θ *off* $1/2$ *when the joint intrinsic measure satisfies the single-partner invariance condition (Theorem 6.2(c)).*

3 Kinematics of the flip motion (Target 14.11 of Article 84)

Article 84's Remark 4.7 and Target 14.11 ask whether the physical motion that executes the flip $\eta_k \mapsto \eta_k + 1$ (and induces $\iota : 3 \leftrightarrow 9, 6 \leftrightarrow 12$ on the primary locants) is an in-plane rotation by the non-trivial element of C_{2h} or an out-of-plane turning-over of the molecular plane [Sch26e]. We settle this unconditionally from Article 40's polyhex classification and the exact Euclidean coordinates of G_{chr}.

Lemma 3.1 (Absence of planar reflections in D_6 and in all of $O(2)$)**. [C], [A]** *In the hexagonal tiling dihedral group* $D_6 = \langle R, S \mid R^6 = S^2 = I, SRS = R^{-1}\rangle$ *of [Sch26a, eqs. (587)–(589)], the canonical chrysene four-cell polyhex* $\mathcal{S}_4 = \{(0,0),(0,1),(1,-2),(1,-1)\}$ *has planar stabilizer* $\Gamma_4^{\mathrm{px}} = \{g \in D_6 : \nu(g\mathcal{S}_4) = \mathcal{S}_4\} = \{I, R^3\} \cong C_2$ *of order 2 ([Sch26a, Table 1, eq. (621)]), containing 0 reflections of* D_6*. Moreover, for the 18-vertex Euclidean carbon skeleton* $\iota_{\mathrm{px}}(V_{\mathfrak{C}}) \subset \mathbb{R}^2$ *of [Sch26a, eqs. (614), (641)–(644)], the centered planar covariance (inertia) tensor* $M = \sum_{v \in V_{\mathfrak{C}}} (\iota_{\mathrm{px}}(v) - c_{\mathrm{mol}})(\iota_{\mathrm{px}}(v) - c_{\mathrm{mol}})^T$ *has exact entries*

$$I_{xx} = 177/8, \qquad I_{yy} = 507/8, \qquad I_{xy} = -91/8\sqrt{3} \neq 0, \quad (1)$$

with strictly distinct eigenvalues $\lambda_\pm = \frac{171 \pm \sqrt{13017}}{4}$*, and reflection across neither principal axis preserves* $\iota_{\mathrm{px}}(V_{\mathfrak{C}})$*. Hence no reflection in the full continuous orthogonal group* $O(2)$ *maps* $\iota_{\mathrm{px}}(G_{\mathrm{chr}})$ *onto itself (Z1).*

Proof. The corrected four cell centers, in the axial convention $X = 3q$, $Y = q + 2r$, have exactly the identity and half-turn in their D_6 stabilizer. The verifier reconstructs these cells from the displayed carbon data and checks the two calculations independently. The original cell list contained a sign error in $(1, 2)$; the consistent entry is $(1, -2)$.

For the continuum group, any orthogonal symmetry fixes the centroid $c_{\mathrm{mol}} = (3/4, -\sqrt{3}/4)$ and commutes with M. Its two distinct eigenspaces leave just two reflection candidates. In centered coefficient coordinates (a, b) with Euclidean point $(a/2, \sqrt{3}b/2)$, these candidates act as

$$\pm \frac{1}{2\sqrt{13017}} \begin{pmatrix} -165 & -273 \\ -91 & 165 \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix}. \quad (2)$$

Every carbon has rational a, b. Since $114^2 < 13017 < 115^2$, the denominator is irrational. The numerator matrix is invertible, so a nonzero rational vector cannot be sent to another rational vector. Thus neither reflection permutes the carbon set. Rotations preserving a planar covariance with distinct eigenvalues can only be I or $-I$, both of which do preserve this set. This establishes the complete planar stabilizer without a floating-point tolerance. □

Theorem 3.2 (Classification of 3D isometries of the chrysene skeleton; Conditional resolution of Target 14.11)**. [A]** *Let* $\hat{\iota}_{\mathrm{px}}(G_{\mathrm{chr}}) \subset \mathbb{R}^2 \times \{0\} \subset \mathbb{R}^3$ *be the canonically embedded chrysene carbon skeleton centered at* $c_{\mathrm{mol}} = 0$ *([Sch26a, eqs. (43), (641)–(644), (690)]).*

(a) Full 3D stabilizer: *The orthogonal point group preserving* $\hat{\iota}_{\mathrm{px}}(G_{\mathrm{chr}})$ *is* $\Pi_{\mathfrak{C}}^{\mathrm{core}} = C_{2h}^{\mathrm{std}} = \{I_3, C_2(z), \sigma_h, -I_3\}$ *of order 4, whose elements have determinants and z-face actions:*

Operation	$\det R$	*Face*	*Locants*
I_3	$+1$	*preserved*	*identity*
$C_2(z)$	$+1$	*preserved*	ι
σ_h	-1	*exchanged*	*identity*
$-I_3$	-1	*exchanged*	ι

(b) No facial turnover in $SO(3)$ preserves the carbon footprint: *The proper rotational stabilizer of* $\hat{\iota}_{\mathrm{px}}(G_{\mathrm{chr}})$ *is* $C_{2h}^{\mathrm{std}} \cap SO(3) = \{I_3, C_2(z)\}$*. No proper rotation* $R \in SO(3)$ *that exchanges the* $+z$ *and* $-z$ *faces (*$Re_z = -e_z$*, i.e.,* 180° *turnover* $R_\pi(\hat{u}_{xy})$ *about any axis* $\hat{u}_{xy}$ *in the molecular plane) maps* $\hat{\iota}_{\mathrm{px}}(G_{\mathrm{chr}})$ *onto itself; every such turnover maps* $\hat{\iota}_{\mathrm{px}}(G_{\mathrm{chr}})$ *to its distinct 2D reflection enantiomorph in* $z = 0$*.*

(c) Physical identification of the flip ([Sch26e, Target 14.11]): *Within* $SO(3)$ *(rigid-body motions), the flip inducing* ι *(*$3 \leftrightarrow 9, 6 \leftrightarrow 12$*) on the canonical chrysene footprint is uniquely the* in-plane half-turn $C_2(z)$*. Realizing* ι *together with facial exchange* $(z \mapsto -z)$ *requires the improper inversion* $-I_3 = C_2(z)\sigma_h \in O(3) \setminus SO(3)$*, which is a symmetry operation rather than a rigid-body trajectory. A molecular pathway relating the resulting arm conformations requires an independent kinetic and steric analysis (Z1).*

Proof. (a) By [Sch26a, App. A.4, eq. (617)], $\Pi_4^{\mathrm{px}} = \langle \Gamma_4^{\mathrm{px}}, \sigma_h \rangle$ where $\Gamma_4^{\mathrm{px}} = \{I, R^3\}$ acts on $\mathbb{R}^2 \times \{0\}$ by I_3 and $C_2(z) = \mathrm{diag}(-1, -1, 1)$, and $\sigma_h = \mathrm{diag}(1, 1, -1)$ fixes every carbon atom in $z = 0$ ([Sch26a, eq. (661)]). Their product $C_2(z)\sigma_h = -I_3$ acts on $z = 0$ identically to $C_2(z)$, hence also induces ι. (b)

Any $R \in SO(3)$ mapping the plane $z = 0$ to itself satisfies $Re_z = \pm e_z$. Since $\det R = +1$, the planar restriction $R|_{z=0} \in O(2)$ has $\det_{2D}(R|_{z=0}) = R_{33} \in \{+1, -1\}$. If R exchanges the $+z$ and $-z$ faces ($R_{33} = -1$), then $R|_{z=0}$ is a 2D reflection in $O(2) \setminus SO(2)$. By Lemma 3.1, no reflection in $O(2)$ preserves $\hat{\iota}_{\mathrm{px}}(G_{\mathrm{chr}})$. (c) Immediate from (a) and (b): in C_{2h}^{std}, the two elements inducing ι are $C_2(z) \in SO(3)$ and $-I_3 \notin SO(3)$. □

Corollary 3.3 (Enantiotopic faces and Article 65's two-sidedness)**. [A]** *An isolated planar chrysene molecule in $z = 0$ is achiral in $\mathbb{R}^3$ ($\sigma_h, -I_3 \in C_{2h}^{\mathrm{std}}$), yet its $+z$ and $-z$ faces are* enantiotopic*: an identical face-specific marker or complexing partner placed in symmetry-related positions above and below the plane gives mirror-related complexes that cannot be superposed by a proper symmetry of the core (Z1). This resolves the apparent tension between [Sch26a, Prop. 2] (C_{2h} is achiral) and [Sch26b, Def. 5.1, Table 1] (which records D, I, T as both achiral and "two-sided—whether the object has distinguishable faces").*

Proof. A planar figure has distinguishable faces under 3D rigid motions in $SO(3)$ iff its 2D symmetry group in $O(2)$ contains no reflection. By Lemma 3.1, $\Gamma_4^{\mathrm{px}} = C_2 \subset SO(2)$ contains no reflection in $O(2)$, whereas in $O(3)$ the improper reflection σ_h fixes $z = 0$, making the 3D object achiral. □

4 Emergent assembly chirality (Theorem 47 of Article 40)

We now give a conditional resolution of [Sch26a, Thm. 47] by computing the Euclidean stabilizer $\Gamma_{\mathfrak{S}}(\eta)$ of a stacked column as a function of its alignment field $\eta \in \{0,1\}^{l-1}$.

Definition 4.1 (Faithful decorated realization)**. [D]** Let $l \geq 2$, $w \in \{0,1\}^l$, and $\eta_i = w_i + w_{i+1} \pmod 2$. The layers have distinct heights kc_z, $c_z > 0$, and a species word $S = (S_0, \ldots, S_{l-1})$. The realization hypothesis H_{real} comprises the following requirements.

(i) The complete decorated assembly, including arms and contact geometry, has an intrinsic layer decomposition preserved by every isometry between members of the realization family. Its induced action is either layer identity or reversal; no axis-mixing isometries are admitted.

(ii) Proper congruence classes are faithfully indexed by (S, η), with global complementation of w a proper change of frame. This faithfulness concerns the full decoration, not the undecorated C_{2h} core.

(iii) A fixed improper reflection maps the class (S, η) to $(\mathrm{rev}\, S, \mathrm{rev}_\eta\, \eta)$. This is an equivariance requirement on the complete geometry, including all chemical labels.

(iv) For the cap extension, the only layer-preserving candidate linear parts are I_3 and $C_2(z)$, and every improper candidate reverses the layers. The asymmetric cap is an actual part of the decorated object, with $\iota I \neq I$.

The earlier contact condition H_{twist} is retained as physical motivation but does not imply these requirements. In particular, asserting that existing symmetries act through the frame group is only a necessary action constraint; it supplies neither faithfulness nor reflection equivariance. Existence of a chemically admissible realization satisfying H_{real} is a separate molecular target.

Lemma 4.2 (Reflection action on the registry quotient)**. [A], [D]** *The agreement map obeys*

$$\begin{aligned} \mathrm{agr}(\mathrm{flip}\, w) &= \mathrm{agr}(w), \\ \mathrm{agr}(\mathrm{rev}\, w) &= \mathrm{rev}_\eta\, \mathrm{agr}(w), \\ (\mathrm{rev}_\eta\, \eta)_i &= \eta_{l-2-i}. \end{aligned} \tag{3}$$

Its fibres are $\{w, \mathrm{flip}\, w\}$. Under H_{real}, an assembly admits an improper self-isometry if and only if its species word and alignment field are both palindromic.

Proof. The identities follow by expanding adjacent binary sums. Given w_0, the recurrence $w_{i+1} = w_i + \eta_i \pmod 2$ reconstructs the unique lift, so the two lifts differ by global complementation. For the geometric statement, let J be the improper reflection in the realization hypothesis. An improper self-isometry exists exactly when $J\mathfrak{S}$ is properly congruent to $\mathfrak{S}$: compose a proper congruence with J in one direction, and an improper self-isometry with J^{-1} in the other. Faithfulness and equivariance identify this equality of proper congruence classes with $(S, \eta) = (\mathrm{rev}\, S, \mathrm{rev}_\eta\, \eta)$. □

Example 4.3 (Why the bare core does not encode the field)**. [A]** For coaxial copies of a planar C_{2h} core with no distinguishing decoration, $C_2(z)$ maps each core onto itself. Changing any w_k therefore leaves the point set unchanged. All binary words then describe the same geometry; the registry count cannot be interpreted as a count of stereoisomers. This example isolates the need for the faithfulness clause of H_{real}.

Theorem 4.4 (Emergent Chirality Classification Theorem; Conditional resolution of Article 40, Theorem 47)**. [D]** *Under H_{real}, let $\mathfrak{S}(\eta)$ be an uncapped stack of length $l \geq 2$ with alignment field $\eta \in \{0,1\}^{l-1}$.*

(a) Palindrome criterion on species-symmetric stacks: *If the species assignment is palindromic ($S_k = S_{l-1-k}$ for all k, including every homotypic column T^l of the interior lattice or D^l of the stock phase), then $\mathfrak{S}(\eta)$ is* achiral in $E(3)$ *($\Gamma_{\mathfrak{S}}(\eta) \cap \{g \in E(3) : \det R_g = -1\} \neq \emptyset$) if and only if η is a palindrome:*

$$\mathrm{rev}_\eta(\eta) = \eta \quad \Longleftrightarrow \quad \eta_i = \eta_{l-2-i} \quad (0 \leq i \leq l-2). \tag{4}$$

Equivalently, $\mathfrak{S}(\eta)$ is chiral *($\Gamma_{\mathfrak{S}}(\eta) \subseteq SE(3)$) if and only if $\mathrm{rev}_\eta(\eta) \neq \eta$, in which case $\mathfrak{S}(\mathrm{rev}_\eta(\eta))$ is its non-superimposable 3D mirror enantiomer. On an even-length alternating cluster $(D,T)^N$ ($S_0 = D \neq T = S_{2N-1}$), $k \mapsto 2N-1-k$ exchanges $D \leftrightarrow T$ so every configuration is chiral under the realization hypothesis in $E(3)$, while (4) characterizes achirality of the alignment field and of the cluster reading under [Sch26d, Def. 4.1, Prop. 4.7] (Remark E.3).*

(b) Bijection with the orbit sizes of the frame group Fr: *The counts in (b)–(c) are combinatorial for every fixed species word; their achiral/chiral interpretation applies only when $S = \mathrm{rev}\, S$. Under the bijection of [Sch26e, Thm. 6.5, Lem. 8.10] between* Fr*-orbits on $\{0,1\}^l$ and $\langle \mathrm{rev}_\eta \rangle$-orbits on $\{0,1\}^{l-1}$:*

- *The* size-2 Fr-orbits *are precisely the palindromic (*achiral registry*) classes, numbering*

$$N_{\mathrm{achiral}}(l) = 2^{\lceil (l-1)/2 \rceil}. \tag{5}$$

- *The* size-4 Fr-orbits *are precisely the non-palindromic enantiomeric-pair classes, numbering*

$$N_{\mathrm{chiral}}(l) = \frac{2^{l-1} - 2^{\lceil (l-1)/2 \rceil}}{2} = N(l) - 2^{\lceil (l-1)/2 \rceil}, \tag{6}$$

covering $2N_{\mathrm{chiral}}(l) = 2^{l-1} - 2^{\lceil (l-1)/2 \rceil}$ chiral alignment fields.

(c) At the corpus's distinguished lengths: *At codon length $l = 6$ ($N(6) = 20$ classes, 32 fields), exactly 8 classes (8 fields) are palindromic* achiral registry *fields and 12 classes (24 fields, forming 12 mirror pairs, or 75.0% of all fields) are chiral. At $l = 12$ ($N(12) = 1,056$), 64 classes are palindromic and 992 are chiral (96.875% of fields); at $l = 16$ ($N(16) = 16,512$), 256 are palindromic and 16,256 are chiral; at $l = 54$, only $134,217,728$ of the 2^{53} fields (fraction 1.49×10^{-8}) are palindromic (Z2, Z3).*

Proof. (a) When $S_k = S_{l-1-k}$, reversal $k \mapsto l-1-k$ preserves the chemical species at every layer, so by Lemma 4.2 an improper Euclidean operation preserves $\mathfrak{S}(\eta)$ iff $\mathrm{rev}_\eta(\eta) = \eta$. On $(D,T)^N$, $S_0 = D \neq T = S_{2N-1}$ forbids $k \mapsto 2N-1-k$ as a chemical symmetry in $E(3)$, while [Sch26d, Def. 4.1] identifies clusters under end-to-end reversal together with the species-offset shift. (b) By [Sch26e, Lem. 8.10], $\mathrm{agr} : \{0,1\}^l \to \{0,1\}^{l-1}$ has fibres $\{w, \mathrm{flip}\, w\}$ of size 2. A $\langle \mathrm{rev}_\eta \rangle$-orbit $\{\eta, \mathrm{rev}_\eta(\eta)\}$ on $\{0,1\}^{l-1}$ is a singleton iff $\mathrm{rev}_\eta(\eta) = \eta$ (giving an Fr-orbit of size $2 \times 1 = 2$) and has size 2 iff $\mathrm{rev}_\eta(\eta) \neq \eta$ (giving an Fr-orbit of size $2 \times 2 = 4$). A palindrome in $\{0,1\}^{l-1}$ is determined by its first $\lceil (l-1)/2 \rceil$ letters, giving (5) and (6). (c) Evaluated in exact integer arithmetic in blocks Z2 and Z3. □

Corollary 4.5 (Racemic endogenous assembly vs. homochiral exogenous placement)**. [D]** *Under H_{real}, on an uncapped species-symmetric blind column of length $l \geq 3$ under [Sch26e, Thm. 7.10(a)]:*

(a) The endogenous draw μ_{endo} produces a non-palindromic chiral field with probability $P_{\mathrm{chiral}}(l) = 1 - 2^{-\lfloor (l-1)/2 \rfloor} \geq \frac{1}{2}$ (75.0% at $l = 6$), but assigns identical mass $\mu_{\mathrm{endo}}(\eta) = \mu_{\mathrm{endo}}(\mathrm{rev}_\eta(\eta)) = 2^{-(l-1)}$ to every chiral field and its mirror enantiomer. Hence the endogenous source is racemic in its ideal ensemble law *(enantiomeric excess* ee = 0% *on every chiral class).*

*(b) The exogenous placed source (H_{place}) prepares a single prescribed η^0 at preparation (*ee = 100% *whenever $\eta^0 \neq \mathrm{rev}_\eta(\eta^0)$). The 1-bit difference between the field selection cost ($l-1$ bits) and the size-4 class selection cost ($l-2$ bits) in [Sch26e, Thm. 9.2, Rem. 9.3] is precisely the* 1 *bit of* enantiomeric selection *choosing between the two chiral enantiomers η^0 and $\mathrm{rev}_\eta(\eta^0)$ inside a size-4 frame class!*

Proof. Part (a) follows from uniformity $\mu_{\mathrm{endo}}(\eta) = 2^{-(l-1)}$ and (6). For (b), by [Sch26e, Thm. 9.2], a class $O \in \{0,1\}^{l-1}/\langle \mathrm{rev}_\eta \rangle$ costs $(l-1) - \log_2 |O|$ bits: on the $N_{\mathrm{achiral}}(l)$ palindromic classes ($|O| = 1$ on fields, $|Orb_{\mathrm{Fr}}| = 2$ on lifts) the field and class costs both equal $l-1$ bits, whereas on the $N_{\mathrm{chiral}}(l)$ chiral classes ($|O| = 2$ on fields, $|Orb_{\mathrm{Fr}}| = 4$ on lifts) the class costs $l-2$ bits and selecting one enantiomer from the pair $\{\eta^0, \mathrm{rev}_\eta(\eta^0)\}$ costs the remaining 1 bit (Z2). □

Remark 4.6 (Population law and persistence)**. [D]** Mirror invariance gives zero ensemble signed excess within each chiral pair, not exact equality in every finite batch. Finite samples fluctuate. A selected geometry remains a useful stereochemical assignment only when its interconversion time is long compared with preparation, observation and storage times. The ideal 100% placed-source value describes a specified initial distribution; neither an achiral cap nor field selection alone establishes a persistent homochiral synthesis.

Scholium 4.7 (The physical meaning of the 8-and-12 split in Article 84). Article 84's Theorem 6.5 recorded that the 20 frame classes of a six-site stack split into 8 orbits of size two and 12 orbits of size four, and its Remark 9.3 noted that the selection cost of a class is 5 bits on the first eight and 4 bits on the other twelve [Sch26e]. Theorem 4.4 and Corollary 4.5 reveal what that combinatorial split is in three-dimensional space: the 8 orbits of size two are the palindromic *achiral registry* stacks (whose mirror image is already the same alignment field, so specifying the class specifies the field at 5 bits), and the 12 orbits of size four are the 12 chiral mirror pairs (where specifying the class up to mirror reversal costs 4 bits, and choosing the right-handed or left-handed enantiomer costs the fifth bit).

5 Initiator capping of columns and the interior lattice (Target 14.14 of Article 84)

We now give a conditional resolution of [Sch26e, Target 14.14]: determining how an initiator unit $I = \{3, 6, 12\}$ caps a column or a face of the $B(3, 3, 6)$ interior lattice to fix its frame and break improper symmetry, and whether Article 79's exported stream supplies enough I units per period.

Theorem 5.1 (Universal chirality of I-capped stacks)**. [D]** *Let a stack of $l \geq 2$ sites carry D or T units at sites $k \in \{1, \dots, l-1\}$ and be capped at site $k = 0$ by the trisubstituted initiator $I = \{3, 6, 12\}$ under H_{frame} and H_{real} ([Sch26e, Hyp. 4.5, Thm. 7.13]). Then:*

(a) Every end-to-end reversing isometry ($k \mapsto l - 1 - k$) is excluded from $\Gamma_\Subset$ by constitutional species asymmetry at the termini ($S_0 = I \neq S_{l-1} \in \{D, T\}$).

(b) The only candidate non-trivial layer-preserving rotation, $C_2(z)$, is excluded from $\Gamma_\Subset$ by locant asymmetry at the cap; layer-preserving improper candidates are excluded by H_{real} ($\iota I = \{6, 9, 12\} \neq I$, point group C_s with no $C_2(z)$ axis and no inversion center; [Sch26g, Rem. 4.3]).

(c) Consequently, the Euclidean stabilizer of the I-capped stack is trivial, $\Gamma_\Subset = \{I_3\} \subset SE(3)$, for all 2^{l-1} alignment fields $\eta \in \{0, 1\}^{l-1}$*: capping converts all $2^{\lceil (l-1)/2 \rceil}$ palindromic* achiral registry *fields into chiral decorated assemblies and distinguishes η from* $\text{rev}_\eta(\eta)$ *as framed decorated configurations when these fields differ (Z4).*

Proof. An element $g \in \Gamma_\Subset$ must preserve the chemical species at each site ([Sch26a, Axiom A_2, eq. (36)]). Since $S_0 = I$ and $S_{l-1} \in \{D, T\}$, g cannot send $k = 0$ to $k = l - 1$, ruling out all reversing maps $z \mapsto (l-1)c_z - z$. Thus g must fix every layer $k \mapsto k$, including $k = 0$. At $k = 0$, $\iota I = \{6, 9, 12\} \neq \{3, 6, 12\} = I$, so neither $C_2(z)$ nor $-I_3$ preserves the cap's substituted locant set, and H_{real} excludes σ_h. Hence $R_g = I_3$ and $t_g = 0$. □

Proposition 5.2 (Stoichiometric sufficiency and bridge compatibility of I-capping on $B(3, 3, 6)$; Conditional resolution of Target 14.14)**. [D]** *Under Article 79's matched design equation $k_3 = e_2(R_T/R_D)(1 + x)$ with $R_D = 42,354$, $R_T = 208$, strand initiator demand $R_I = c_I = 1$, and $x = e_3/k_4 > 0$ ([Sch26g, Thm. 7.2, Cor. 7.4, Def. 10.1]):*

(a) Initiator cap budget: *At minimum bulk throughput $\Phi_{\min} = R_D/p_2 = R_T/p_4$, the source exports $\Phi_{\min} p_3 = R_T x = 208x$ initiator units per period, leaving a net cap surplus after strand polymerization of*

$$\Delta N_I(x) := \Phi_{\min} p_3 - R_I = 208x - 1. \tag{7}$$

At Article 79's baseline $x = 0.1$, $\Phi_{\min} p_3 = 20.8$ and $\Delta N_I(0.1) = 19.8$ units per period (Z5).

(b) Sufficiency for the $B(3, 3, 6)$ heritable lattice: *In Article 80's $B(3, 3, 6)$ lattice (9 vertical columns of height 6, with 1 central complete column $(1, 1, k_z)$) [Sch26c]:*

- *Capping the central complete column requires 1 unit ($\Delta N_I(x) \geq 1 \iff x \geq 1/104 \approx 0.00962$).*
- *Capping all 9 columns of the 3×3 basal face $k_z = 0$ requires 9 units ($\Delta N_I(x) \geq 9 \iff x \geq 5/104 \approx 0.04808$).*
- *Capping two complete lattices in the Type B inheritance route of [Sch26c, Cor. 5.4] (or, as a resource count only, both faces of one Type A lattice) requires 18 units ($\Delta N_I(x) \geq 18 \iff x \geq 19/208 \approx 0.09135 \leq 0.1$).*

All three demands are met out of the existing 19.8-unit surplus at $x = 0.1$ in the loss-free mean-throughput ledger, with zero increase in $\Phi_{\min}$ and unchanged model bulk efficiency $\eta = 0.998437$.

(c) Exact lateral-bridge compatibility on the $k_x \in \{0, 2\}$ boundaries: *In $B(3, 3, 6)$, a node at (k_x, k_y, k_z) requires an arm at locant $9 = v_x^+$ iff $k_x \in \{0, 1\}$, and at locant $3 = v_x^-$ iff $k_x \in \{1, 2\}$ (the free-arm characterization in Article 90 [Sch26f]). Since $I = \{3, 6, 12\}$ ($w_0 = 0$) lacks an arm only at $9 = v_x^+$ and its $C_2(z)$-rotated state $\iota I = \{6, 9, 12\}$ ($w_0 = 1$) lacks an arm only at $3 = v_x^-$, placing I ($w_0 = 0$) at the 3 columns $(2, k_y, 0)$ and ιI ($w_0 = 1$) at the 3 columns $(0, k_y, 0)$ (6 of the 9 basal columns in total), or capping any column at an unbridged overhang $k_z = -1$, satisfies saturated bridging H_{sat} across every incident lateral connector without a single missing bridge (Z5).*

The numerical throughput is an expected resource flux, not a deterministic integer yield in every period. For full nine-column capping, the three $k_x = 1$ columns require unbridged external overhangs; substituting I for a saturated in-layer central T would remove a required lateral port. The one-ended chirality theorem does not cover identically capped two-ended columns, whose reversal symmetry must be analyzed separately. These distinctions separate resource feasibility from connector compatibility and from molecular cap formation.

Proof. (a) By [Sch26g, Prop. 6.9], $p_3/p_4 = e_3/k_4 = x$, and $\Phi_{\min} = R_T/p_4$, so $\Phi_{\min} p_3 = R_T(p_3/p_4) = R_T x = 208x$. Subtracting $R_I = 1$ gives (7). (b) Solving $208x - 1 \geq m$ for $m \in \{1, 9, 18\}$ gives $x \geq 2/208, 10/208, 19/208$, all strictly below $x = 0.1$ where $\Delta N_I(0.1) = 19.8$. (c) By [Sch26a, eqs. (50)–(51), (107)], locant $3 = v_x^-$ bridges to $k_x - 1$, locant $9 = v_x^+$ bridges to $k_x + 1$, locant $12 = v_y^-$ bridges to $k_y - 1$, and locant $6 = v_y^+$ bridges to $k_y + 1$. At $k_x = 2$, v_9 is unbridged so $\{3, 6, 12\} = I$ supplies all three interior bridges; at $k_x = 0$, v_3 is

unbridged so $\{6, 9, 12\} = \iota I$ supplies all three interior bridges (Z5). □

6 Out-of-plane arm conformations and contact bias (Target 14.1 of Article 84)

Article 84's Target 14.1 asks whether a stacking contact between delivered $D(ee)$ or $T(eeee)$ units acquires an orientation bias $\theta \neq 1/2$ from non-centrosymmetric or out-of-plane arm conformations [Sch26e]. We now derive the exact symmetry condition governing that bias across all conformational states.

Definition 6.1 (Out-of-plane arm sign configurations)**. [A]** For a unit with ι-invariant family $S \in \{D, T\}$ and constant arm word $e^{|S|}$, let $\zeta : S \to \{+1, -1\}$ record whether the terminal of the flexible arm at locant $l \in S$ is displaced into the $+z$ or $-z$ half-space relative to the chrysene plane. Under the generators of C_{2h}^{std} (Theorem 3.2(a)):

$$\begin{aligned}(C_2(z)\zeta)(l) &= \zeta(\iota l),\\ (\sigma_h\zeta)(l) &= -\zeta(l),\\ (-I_3\zeta)(l) &= -\zeta(\iota l).\end{aligned} \tag{8}$$

These are coarse sign decorations. The stabilizers below are subgroups of the core group acting on this finite sign set. An atomistic conformer has the same point group only if its full coordinates realize the sign decoration equivariantly and have no further symmetry-breaking features. Arm lengths, torsions, solvent and bonding are not reconstructed by a sign vector.

Here syn and anti refer only to relative terminal half-space signs, not complete atomistic stereodescriptors. Call ζ *C_2-symmetric (syn)* if $\zeta(\iota l) = +\zeta(l)$ for all $l \in S$, *C_i-symmetric (anti / centrosymmetric)* if $\zeta(\iota l) = -\zeta(l)$ for all $l \in S$, and *C_1 (mixed)* on T if one ι-orbit is syn and the other is anti.

Theorem 6.2 (Conformational classification and contact-bias mechanism; Addressing Target 14.1)**. [A]** *Let $\zeta \in \{+1, -1\}^S$ range over the out-of-plane sign configurations of $D(ee)$ and $T(eeee)$.*

(a) Conformational symmetry partition:

- *On $D = \{6, 12\}$ (4 states): 2 states are C_2-symmetric ($\{(+,+),(-,-)\}$, mirror-related sign states exchanged by σ_h and $-I_3$, fixed by $C_2(z)$) and 2 states are C_i-symmetric ($\{(+,-),(-,+)\}$, centrosymmetric sign states fixed by $-I_3$ and exchanged by $C_2(z)$ and σ_h).*
- *On $T = \{3, 6, 9, 12\}$ (16 states): 4 states are C_2-symmetric, 4 are C_i-symmetric, and 8 have trivial stabilizer C_1 (one orbit syn, one orbit anti; Z6).*

(b) How locked C_i (anti) and C_1 (mixed) conformers break in-plane $C_2(z)$ blindness: *Suppose two stacked units carry fixed conformational states $\zeta_1 = \zeta_2 = \zeta$ and interact via the pairwise contact energy $E_\eta(\zeta, \zeta) = -\epsilon_{\mathrm{syn}} \sum_{l \in S} \zeta(l)\,(C_2(z)^\eta\zeta)(l)$ ($\epsilon_{\mathrm{syn}} \neq 0$). Let $n_{\mathrm{anti}}(\zeta) \in \{0, 1, 2\}$ denote the number of ι-orbits of S on which $\zeta(\iota l) = -\zeta(l)$. Then:*

$$\begin{aligned}\Delta E(\zeta) &:= E_1(\zeta, \zeta) - E_0(\zeta, \zeta)\\ &= 4n_{\mathrm{anti}}(\zeta)\epsilon_{\mathrm{syn}},\\ \theta_{\mathrm{conf}}(\zeta) &= \frac{1}{1 + e^{\Delta E(\zeta)/(k_B T)}}.\end{aligned} \tag{9}$$

In particular: (i) on every C_2 (syn) state ($n_{\mathrm{anti}} = 0$), $\Delta E = 0$ and the contact is strictly blind ($\theta = 1/2$); (ii) on every C_1 mixed state of T ($n_{\mathrm{anti}} = 1$), $\Delta E = 4\epsilon_{\mathrm{syn}}$; and (iii) on every centrosymmetric C_i (anti) state ($n_{\mathrm{anti}} = |S|/2$), $C_2(z)\zeta_{\mathrm{anti}} = -\zeta_{\mathrm{anti}}$ reverses every arm sign, giving maximal bias $\Delta E = 2|S|\epsilon_{\mathrm{syn}}$ ($4\epsilon_{\mathrm{syn}}$ on D, $8\epsilon_{\mathrm{syn}}$ on T).

(c) Annealed restoration under single-partner invariance: *For $C = C_2(z)$ acting on signs, put*

$$\begin{aligned}E_\eta(\zeta_1, \zeta_2) &= -\epsilon_{\mathrm{syn}} \sum_{a \in S} \zeta_1(a)(C^\eta\zeta_2)(a),\\ Z_\eta &= \sum_{\zeta_1, \zeta_2} \rho(\zeta_1, \zeta_2) e^{-E_\eta(\zeta_1, \zeta_2)/(k_B T)}.\end{aligned} \tag{10}$$

Assume $T > 0$, nonnegative nonzero intrinsic weights ρ, equal registry prior weights, and

$$\rho(\zeta_1, C\zeta_2) = \rho(\zeta_1, \zeta_2). \tag{11}$$

Then $Z_0 = Z_1$ and the annealed registry probability is $1/2$. Independent intrinsic measures with a C-invariant second marginal suffice. Symmetry of both one-unit marginals without the joint condition does not suffice.

Proof. (a) On S, ι has $r = |S|/2$ two-element orbits ($r = 1$ on D, $r = 2$ on T). On each orbit, ζ is either syn ($\zeta(\iota l) = +\zeta(l)$, 2 choices) or anti ($\zeta(\iota l) = -\zeta(l)$, 2 choices). Having all r orbits syn gives 2^r C_2 states; having all r orbits anti gives 2^r C_i states; on T ($r = 2$), having one syn and one anti gives $2 \times 2 \times 2 = 8$ C_1 states. (b) At $\eta = 0$, $\sum_{l \in S} \zeta(l)^2 = |S|$, so $E_0 = -|S|\epsilon_{\mathrm{syn}}$. At $\eta = 1$, each syn orbit contributes $+2$ to $\sum \zeta(l)\zeta(\iota l)$ and each anti orbit contributes -2, so $E_1 = -(|S| - 4n_{\mathrm{anti}}(\zeta))\epsilon_{\mathrm{syn}}$, giving $\Delta E = E_1 - E_0 = 4n_{\mathrm{anti}}(\zeta)\epsilon_{\mathrm{syn}}$ and (9). (c) Since $C^2 = 1$, $E_1(\zeta_1, \zeta_2) = E_0(\zeta_1, C\zeta_2)$. Reindex the second sum by $\zeta_2' = C\zeta_2$ and apply (11); this gives $Z_1 = Z_0$. This argument transforms one partner only, not a correlated pair simultaneously. □

Example 6.3 (Correlated anti states retain bias)**. [A]** On D, let $a = (+1, -1)$ and put probability $1/2$ on each pair (a, a) and $(-a, -a)$. Each marginal is invariant under C, but the joint measure is not invariant under $(\zeta_1, \zeta_2) \mapsto (\zeta_1, C\zeta_2)$. Both supported pairs have $E_0 = -2\epsilon_{\mathrm{syn}}$ and $E_1 = 2\epsilon_{\mathrm{syn}}$. Thus $Z_1/Z_0 = e^{-4\epsilon_{\mathrm{syn}}/(k_B T)}$, which differs from one for $\epsilon_{\mathrm{syn}} \neq 0$. Thermal equilibration restores blindness only when the ensemble and timescale assumptions establish the required joint invariance.

Remark 6.4 (Energy and probability interpretation)**. [D]** The coupling ϵ_{syn} has units of energy and its sign is an input of this pair model. The logistic expression is the equilibrium probability of registry $\eta = 1$ for fixed conformers with equal registry priors, not a universal measured stacking rate. A molecular prediction requires calibrated free energies and a separation between conformer relaxation, registry exchange, and assembly timescales.

Scholium 6.5 (A centrosymmetric sign state gives a model contact bias). Theorem 6.2(b) uncovers a striking geometric inversion of expectations for [Sch26e, Target 14.1]. Article 84's Falsification Register suggested that a contact free energy might depend on orientation through a "non-centrosymmetric arm conformation" [Sch26e, §12]. Theorem 6.2(b) proves that under the in-plane $C_2(z)$ flip of Theorem 3.2, it is the *centrosymmetric (C_i, anti)* arm conformation $\zeta_{\text{anti}} = (+1, -1)$ that breaks $C_2(z)$ symmetry ($C_2(z)\zeta_{\text{anti}} = -\zeta_{\text{anti}}$) and generates the maximal orientation bias (9), whereas the non-centrosymmetric C_2 (syn) conformation $\zeta_{\text{syn}} = (+1, +1)$ is fixed by $C_2(z)$ and remains completely blind!

7 Precedence rulings and targets

Ruling 7.1 (Articles 40, 65, 79, 80, and 84)**. [D]** Consistent; conditional extensions of one deferred theorem of Article 40 and three targets of Article 84:

(i) *Article 40, Theorem 47 (Emergent Chirality Theorem):* Addressed under the stated hypotheses by Lemma 4.2 and Theorem 4.4. An uncapped species-symmetric stack under H_{real} is chiral iff its alignment field $\eta \in \{0, 1\}^{l-1}$ is non-palindromic ($\text{rev}_\eta(\eta) \neq \eta$), corresponding to the size-4 orbits of Fr.

(ii) *Article 65, Table 1 and Article 40, Proposition 2 (Two-sidedness vs. Achirality):* Reconciled by Lemma 3.1, Theorem 3.2, and Corollary 3.3. The isolated core is 3D-achiral in $O(3)$ ($\sigma_h \in C_{2h}^{\text{std}}$) while possessing enantiotopic faces in $SO(3)$ (zero reflections in $O(2)$).

(iii) *Article 84, Target 14.11 (The flip motion):* Addressed under the stated hypotheses by Theorem 3.2. Within $SO(3)$ on the canonical polyhex footprint, the flip is the in-plane half-turn $C_2(z)$; facial turnover inducing ι is $-I_3 \in O(3) \setminus SO(3)$.

(iv) *Article 84, Target 14.14 (Frame carrier in the lattice):* Addressed under the stated hypotheses by Theorem 5.1 and Proposition 5.2. Article 79's 19.8-unit initiator surplus caps up to 19 columns per period, covering the 9 columns of $B(3, 3, 6)$ with full in-layer bridge compatibility on the 6 boundary columns $k_x \in \{0, 2\}$.

(v) *Article 84, Target 14.1 (Orientation bias):* Addressed by Theorem 6.2, establishing $\Delta E = 4n_{\text{anti}}(\zeta)\epsilon_{\text{syn}}$ across all C_2, C_i, and C_1 conformers.

Target 7.2 (Structural and chiroptical tests of the decorated realization)**.** Establish complete coordinates, connectivity, species assignment and orientation-sensitive decoration before identifying a registry field with a stereoisomer. Compare enantiomer-resolved preparations with racemate and achiral controls. In an achiral environment, mirror-related preparations should give opposite circular-dichroism spectra where the signal is nonzero, while ideal equal populations cancel. Chirality does not require a detectable band at every wavelength, and a null spectrum alone does not prove an achiral structure. Check concentration and aggregation dependence, configurational persistence, and linear-dichroism or scattering artifacts in oriented samples. Terminology follows the IUPAC stereochemical recommendations [Mos96].

Target 7.3 (Rotational vs. conformational barrier of $\zeta_{\text{anti}} \leftrightarrow -\zeta_{\text{anti}}$)**.** Compute a defined interconversion pathway and free-energy barrier, or use variable-temperature NMR when exchanging states give distinguishable signals, for the transition between the two C_i (anti) arm conformations $(+1, -1)$ and $(-1, +1)$ of $D(ee)$ inside an aqueous column separately from the model equilibrium contact-energy difference $4\epsilon_{\text{syn}}$ of Theorem 6.2(b).

8 Conclusion

The canonical C_{2h} core has enantiotopic faces and an in-plane half-turn as its only proper locant-flip symmetry. Exact binary enumeration yields 8 palindromic fields and 12 non-palindromic reversal pairs at length six. Under a faithful reflection-equivariant decorated realization, those become achiral assemblies and chiral mirror pairs. The separation between enumeration and realization is essential because the undecorated half-turn-symmetric core cannot distinguish the binary orientations. A unique asymmetric terminal cap eliminates the admitted nonidentity column symmetries, while the imported source model supplies sufficient mean resources for the stated cap budgets. Full-face cap geometry, molecular attachment and retention remain distinct requirements. Finally, the reduced arm-sign energy model gives an explicit locked-conformer bias and an annealed blindness theorem under single-partner joint invariance, with a correlated counterexample showing the sharp distinction. These results provide exact mathematical criteria and testable molecular targets for the next stage of the framework.

Table 1: Core kinematics and conditional decorated-assembly classification under H_{real}. Population percentages describe ideal laws, not guaranteed finite batches.

Assembly Stage	Point / Space Stabilizer	Chirality & Source Status	Unified Theorem & Stoichiometry
1. Isolated planar core (D, T)	$\Pi_{\mathfrak{C}}^{\text{core}} = C_{2h}^{\text{std}} = \{I_3, C_2(z), \sigma_h, -I_3\}$ ([Sch26a, Prop. 53])	**3D-achiral** ($\sigma_h, -I_3$ improper), but **enantiotopic faces** ($\Gamma_4^{\text{px}} = C_2$ has 0 reflections in $O(2)$)	Flip ι in $SO(3)$ is uniquely $C_2(z)$; facial exchange with the same locant action uses improper $-I_3$; addresses conditionally [Sch26e, Target 14.11] (Lem. 3.1, Thm. 3.2)
2. Uncapped *achiral registry* stack ($\eta = \text{rev}_\eta(\eta)$)	Contains an improper self-isometry under H_{real} for species-symmetric stacks	**Achiral (*achiral registry*)**: $N_{\text{achiral}}(l) = 2^{\lceil (l-1)/2 \rceil}$ classes (8 classes, 8 fields at $l = 6$)	Bijects with size-2 Fr-orbits; field and class selection costs both equal $l - 1$ bits (Thm. 4.4, Cor. 4.5)
3. Uncapped chiral stack ($\eta \neq \text{rev}_\eta(\eta)$)	$\Gamma_{\Im}(\eta) \subseteq SE(3)$ ($\det R_g = +1$ only)	**Chiral**: $N_{\text{chiral}}(l) = \frac{2^{l-1} - 2^{\lceil (l-1)/2 \rceil}}{2}$ mirror pairs (12 classes, 24 fields = 75.0% at $l = 6$)	Addresses conditionally [Sch26a, Thm. 47]; μ_{endo} is racemic (ee = 0%); H_{place} selects 1 enantiomer (ee = 100%) for 1 bit (Thm. 4.4, Cor. 4.5)
4. I-capped column	$\Gamma_{\Im} = \{I_3\}$ (species breaks rev; $\iota I \neq I$ breaks $C_2(z), -I_3$)	**100% Chiral**: all 2^{l-1} alignment fields are strictly chiral and constitutionally oriented	Addresses conditionally [Sch26e, Target 14.14]; 19.8 I surplus caps 9 columns of $B(3, 3, 6)$; 6 boundary cols ($k_x \in \{0, 2\}$) fit in-layer (Thm. 5.1, Prop. 5.2)
5. Out-of-plane sign-state model $\zeta \in \{\pm 1\}^S$	$D(ee)$: 2 C_2 + 2 C_i; $T(eeee)$: 4 C_2 + 4 C_i + 8 C_1	Locked C_i and C_1 states have $\Delta E = 4n_{\text{anti}}\epsilon_{\text{syn}}$, giving bias $\theta_{\text{conf}} \neq 1/2$	Addresses [Sch26e, Target 14.1]; joint invariance (11) restores annealed blindness $\theta = 1/2$ (Thm. 6.2)

A Hypothesis register

H_{real}
: Intrinsic layers, faithful proper-congruence classes, mirror equivariance, and complete cap candidate constraints (Definition 4.1). Used for the geometric classification and capped-column conclusion. If it fails, the core kinematics, word counts and sign-state algebra remain valid, but their molecular chirality interpretation need not.

$H_{\text{draw}}, H_{\text{place}}, H_{\text{frame}}$
: Uniform independent endogenous draws, ideal placement and an actual asymmetric cap reference. Used for source weights and cap interpretation. Their failure does not alter the finite enumeration; population and retention conclusions must be recomputed.

$H_{\text{kin}}, H_{\text{sat}}$
: Imported matched kinetics and fixed directional connector incidence. Used for resource throughput and allowed in-layer placements. The identity $\Delta N_I = R_T x - R_I$ remains a conditional ledger formula; measured flux and capture need not equal it.

Pair-energy and annealed premises
: The specified bilinear energy, $T > 0$, equal registry priors and joint single-partner invariance (11). Used for the logistic and annealed probabilities. Locked energy differences remain algebraic within the chosen energy model, but symmetric one-unit marginals alone do not imply blindness.

B Canonical coordinate certificate

The regular carbon model uses $(x, y) = (X/2, \sqrt{3}Y/2)$ and the following exact coefficient pairs, which define the numerical certificate independently of the imported polyhex notation:

$$\begin{aligned} V_{\text{per}} = \{&(-2, 2), (-1, 3), (1, 3), (2, 2),\\ &(4, 0), (5, -1), (5, -3), (4, -4),\\ &(2, -4), (1, -3), (-1, -1), (-2, 0)\}, \\ V_{\text{fus}} = \{&(-1, 1), (1, -1), (1, 1),\\ &(2, -2), (2, 0), (4, -2)\}. \end{aligned} \tag{12}$$

The perimeter pairs occur in locant order $1, \ldots, 12$. The centroid in coefficient coordinates is $(3/2, -1/2)$; the physical centroid and covariance follow by the stated embedding. This is an idealized geometric model, not a crystallographic measurement. The corrected covariance supersedes the inconsistent values in the supplied draft and historical review.

C Verification blocks

Quantitative macros in the body are emitted by `verify_a91.py` (Python standard library; exact integer and rational arithmetic). The imported values p_3 and η_{total} remain explicitly tagged model inputs, not experimentally verified quantities. The new code uses checks that remain active under Python optimization; the companion proof document states the precise finite Lean coverage. The seven verification blocks are:

Z1 Polyhex D_6 stabilizers, continuum $O(2)$ inertia tensor, and 3D flip kinematics.
Applies all 12 elements of D_6 to the corrected four-cell chrysene footprint and independently checks the supplied 18 carbon coordinates, confirming $|\Gamma_4^{\mathrm{px}}| = 2$ with 0 reflections on $\mathcal{S}_4$; computes the exact centered inertia tensor $I_{xx} = 177/8, I_{yy} = 507/8, I_{xy} = -91/8\sqrt{3} \neq 0$ on the 18 carbon vertices of G_{chr} to exclude off-lattice reflections in $O(2) \setminus D_6$; and verifies that in $O(3)$, $C_2(z)$ and $-I_3$ induce ι while no $R \in SO(3)$ with $R_{33} = -1$ preserves the carbon skeleton (Lemma 3.1, Theorem 3.2, Corollary 3.3). Exact.

Z2 Equivariance and emergent chirality enumeration at $l \leq 14$.
Enumerates all 2^l site words and 2^{l-1} alignment fields for $2 \leq l \leq 14$, verifying (3) and confirming that size-2 Fr-orbits coincide 1-to-1 with palindromic fields ($\mathrm{rev}_\eta(\eta) = \eta$, count $2^{\lceil (l-1)/2 \rceil}$) and size-4 Fr-orbits coincide 1-to-1 with chiral enantiomeric pairs ($\mathrm{rev}_\eta(\eta) \neq \eta$), reproducing $(8, 12)$ classes and $(8, 24)$ fields (75.0%) at $l = 6$ (Theorem 4.4, Corollary 4.5). Exact.

Z3 Closed-form chirality evaluation at $l = 12, 16, 54$.
Evaluates $N(l), N_{\mathrm{achiral}}(l), N_{\mathrm{chiral}}(l)$ at $l = 12$ $(1,056, 64,992, 96.875\%)$, $l = 16$ $(16,512, 256, 16,256)$, and $l = 54$ $(134,217,728$ achiral fields, achiral fraction $1.49 \times 10^{-8})$. Exact.

Z4 Trivial stabilizer of l-capped stacks.
For $2 \leq l \leq 8$, tests all candidate operations in Fr and C_{2h}^{std} on a stack with $S_0 = \{3, 6, 12\}$ and $S_{l-1} \in \{D, T\}$, confirming that only the identity preserves both the terminal species assignment and the cap locant set I across all 2^{l-1} alignment fields (Theorem 5.1). Exact.

Z5 Initiator cap stoichiometry and $B(3, 3, 6)$ dual boundary compatibility.
Computes $\Phi_{\min} p_3 = 20.8$ and $\Delta N_I(x) = 208x - 1 = 19.8$ in exact rational arithmetic from Article 79's parameters, solves the thresholds $x_{\min} = 1/104, 5/104, 19/208$ for $1, 9, 18$ caps, and verifies that on $B(3, 3, 6)$ the 3 columns at $k_x = 2$ fit $I = \{3, 6, 12\}$ and the 3 columns at $k_x = 0$ fit $\iota I = \{6, 9, 12\}$ (6 columns in total) without missing any lateral bridge (Proposition 5.2). Exact.

Z6 Out-of-plane arm conformation orbits.
Enumerates $\zeta \in \{\pm 1\}^S$ under C_{2h}^{std} action (8), confirming $(2, 2)$ (C_2, C_i) states on $D(ee)$ and $(4, 4, 8)$ (C_2, C_i, C_1) states on $T(eeee)$ (Theorem 6.2(a)). Exact.

Z7 Contact bias on locked C_i and C_1 conformers vs. thermal averaging.
Verifies $\Delta E(\zeta) = 4 n_{\mathrm{anti}}(\zeta) \epsilon_{\mathrm{syn}}$ across all 4 states of $D(ee)$ and all 16 states of $T(eeee)$ under $C_2(z)$, and verifies single-partner energy-histogram exchange under invariant pair weights, together with the correlated anti-state counterexample (Theorem 6.2(b)–(c)). Exact.

D Molecular commentary, isolated

Remark D.1 (Status)**. [A]** Nothing in this appendix enters a numbered statement or proof of the main text.

Remark D.2 (2D prochirality and planar chirality in supramolecular stacks)**. [E]** In stereochemistry, a planar molecule with point group C_{2h} (such as *trans*-1,2-dichloroethene or chrysene) is achiral in three-dimensional solution because an improper self-symmetry exists; equivalently its mirror image is superposable by a proper rigid motion. However, when adsorbed onto a surface or confined within a face-to-face π-stack, out-of-plane tumbling can disrupt stacking contacts, with the barrier depending on the actual interface. Because chrysene's planar rotation-and-reflection stabilizer is C_2 rather than one containing reflection lines (in contrast to pyrene $\mathcal{S}_5$ or tetracene $\mathcal{S}_1$ in [Sch26a, Table 1], both of which are D_{2h} and have planar mirror lines), its two faces are enantiotopic (2D-prochiral). Theorem 3.2 shows that this absence of planar reflection symmetry is a direct consequence of Article 40's unique C_{2h} selection among the seven four-ring polyhexes.

Remark D.3 (Why the initiator surplus of Article 79 is not waste)**. [E]** In Article 79's Corollary 7.4, matching the disubstituted and tetrasubstituted streams at $x = e_3/k_4 = 0.1$ produces $\Phi_{\min} p_3 = 20.8$ initiator units per period, whereas the material ledger of Article 65 charges only $R_I = c_I = 1$ initiator unit per period for strand polymerization [Sch26b, Sch26g]. In Article 79, the remaining 19.8 units were treated merely as a harmless 0.05% surplus tolerated to keep the cooperativity ratio $k_4/k_3 = 18,511$ finite. Proposition 5.2 shows that this 19.8-unit pool exceeds the idealized stoichiometric demand to cap the 9 columns of the $B(3, 3, 6)$ interior chrysene lattice (or 18 columns for two Type B daughter lattices). This is a resource-feasibility result under the imported kinetic model. Capture, localization, attachment chemistry and persistence of the cap require independent realization and kinetic evidence.

E What was set aside in preparing this paper

Remark E.1 (Facial turnover as a proper symmetry of the core)**. [A]** An initial intuition in reading [Sch26e, Rem. 4.7] was that rotating a planar chrysene core by 180° around one of its in-plane principal axes (a facial turnover in $SO(3)$) would carry the carbon skeleton onto itself while exchanging $+z \leftrightarrow -z$ and inducing ι. Block Z1 refuted that assumption both in D_6 and in the continuous group $O(2)$: every 180° rotation about an axis

in $z = 0$ acts on the plane $z = 0$ as a 2D reflection, and by Lemma 3.1 chrysene has no planar reflection symmetry even along its principal inertia axes. Turning a chrysene core over in $SO(3)$ changes the handedness of its bay regions in the plane, so the only proper rotation in $SO(3)$ that preserves the canonical carbon footprint and induces ι is the in-plane half-turn $C_2(z)$.

Remark E.2 (Expecting non-centrosymmetric arm conformers to drive the $C_2(z)$ bias)**. [A]** In addressing [Sch26e, Target 14.1], it was initially expected that the chiral, non-centrosymmetric syn conformers $\zeta_{\text{syn}} = (+1, +1)$ on $D(ee)$ would break contact blindness under an in-plane flip. Direct calculation in Theorem 6.2(b) showed the opposite: ζ_{syn} has point group C_2 aligned with $C_2(z)$, so $C_2(z)\zeta_{\text{syn}} = \zeta_{\text{syn}}$ ($n_{\text{anti}} = 0$) and its contacts are completely blind to in-plane rotation; it is the achiral, centrosymmetric anti conformer $\zeta_{\text{anti}} = (+1, -1)$ (point group C_i, $n_{\text{anti}} = 1$) and the 8 mixed C_1 conformers on $T(eeee)$ that change sign under $C_2(z)$ and generate the orientation bias (9).

Remark E.3 (Species parity on even-length alternating clusters vs. homotypic columns)**. [A]** A first draft of Theorem 4.4(a) stated the palindrome criterion $\text{rev}_\eta(\eta) = \eta$ without distinguishing species-symmetric columns ($S_k = S_{l-1-k}$, such as T^l or D^l) from even-length alternating clusters $(D, T)^N$ ($l = 2N$). On $(D, T)^N$, spatial reversal $k \mapsto 2N - 1 - k$ exchanges $D \leftrightarrow T$ at every layer, so no improper Euclidean isometry fixes the chemical species assignment unless accompanied by the species-offset shift of [Sch26d, Def. 4.1]. Theorem 4.4(a) now states both cases explicitly.

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