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Axiom-Free Invariants of the Cut-Set Lattice in the Chrysene Formalism: Admissible Maximal Chains, Obstruction Functionals, and Disjoint Optima on Hamiltonian Paths

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Abstract

This paper characterizes the combinatorial and redox invariants governing the stepwise linearization of the chrysene skeleton, defining the cleavage poset of a chain-forming cut set — whose maximal chains represent the cleavage orderings — to establish how substituent placement and ring-opening sequence determine synthetic pathway properties. Two functionals on this poset structure the analysis: an activation index that counts cleavage steps at unhydrogenated carbons, and the oxidation number, which acts as a path-independent state function that fixes total redox demand directly from the endpoint structures.
Because the chrysene skeleton has an automorphism group of order 2, its two K-regions lie in a single symmetry orbit that is preserved under 6, 12-disubstitution, meaning that ring opening at positions 11–12 and 5–6 represents a single experimental equivalence class. Of the 27 chain-forming cut sets, 24 admit a clean ordering, while the remaining sets are characterized precisely as those in which every bond joins two ring-fusion carbons. Across all cut sets and clean orderings, the activation index has an exact lower bound of 2, which is attained on the poset.
Evaluating where the substituted carbons land along the product chain reveals a structural trade-off between activation count and terminal substituent placement. Exactly 1 of the 7 realized substituent patterns places a substituted carbon at a chain terminus as required for the target 1-yl membrane lipid, and every cut set realizing this terminal pattern carries an activation index of 3. Consequently, minimizing the activation index and delivering the terminal-linkage product are optimized by disjoint families of cut sets separated by 1 step, confirming that the 3-step sequence is optimal for the target lipid architecture. Extending the enumeration across all 5 four-ring cata-condensed isomers — including the branched isomer — shows that all 5 share the minimum activation index of 2 and the clean cut-set count of 24, while chrysene uniquely minimizes the total number of clean orderings. Finally, because the oxidation number is a state function, reaching the target ether lipid chain requires 52 reducing equivalents per dimer independently of mechanism, confirming the route-based material ledger directly from the molecular endpoints.

Keywords: Chrysene Formalism; cleavage poset; cut set; clean ordering; activation obstruction; graph automorphism; cata-condensed benzenoid; oxidation number; state function

1 Introduction

Article 62 [1] enumerated the cut sets of the chrysene skeleton and computed a lipid from one of them. Article 83 [2] took the resulting membrane and scored it against invariants fixed in advance from the measured literature, and in the course of doing so established a sequential model for the cleavage itself: a theorem on which orderings of a cut set are *clean*, in the sense that no step cuts a bond interior to a fused system of the substrate as it then stands. That theorem reported that 24 of 27 openings admit such an ordering, and it reported an obstruction alongside: at two to three of the four steps neither carbon of the bond being cut bears a hydrogen, which blocks the catechol-type activation its imported reaction class uses.

Article 83 left the obstruction as a feature of the route it was describing. The question this article asks is whether it is one. The answer is that it is not: it is a property of the skeleton, and no choice of cut set or ordering removes it.

Getting to that answer requires naming an object Article 83 left implicit. A cut set is a set of four bonds; an ordering is a sequence of them; and the states in between form a poset whose maximal chains are the orderings. Section 4 sets this out and puts two functions on it. The first, the activation index, counts the steps at which neither carbon bears a hydrogen *at the moment of cleavage* — the qualification matters, because cleaving a bond caps the two carbons it joined, so a step may inherit a hydrogen the parent did not supply, and the index is consequently smaller than a count over bond classes would predict. The second, the oxidation number, is a state function, so the redox demand of a route depends only on its endpoints.

Sections 5 to 7 establish the combinatorics: an exact characterisation of which cut sets admit a clean ordering, and the

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bound $\alpha_{\min} \geq 2$. Section 8 is the article's main result and was not anticipated when the computation was begun. Every cut set delivers the same C_{18} carbon skeleton, so what distinguishes them is where the two substituted carbons land along the product chain. The Article 62 lipid is a di-*O*-(octadec-9-en-1-yl) phosphate, and the 1-yl places its linkage carbon at a chain terminus. Exactly one of the 7 patterns realised has a substituted carbon at a terminus, and every cut set realising it carries activation index 3 rather than the floor 2. The two desiderata are optimised by disjoint families of cut sets, separated by exactly 1 step. The practical reading is the reverse of what Theorem 7.1 alone would suggest: the sequence recorded for the experimental programme is optimal given the product, and the extra obstructed step is the price of the lipid rather than a defect in the choice.

Section 9 repeats the enumeration on the other four four-ring cata-condensed isomers of the same formula — three chains and one branched — to separate facts about chrysene from facts about its family. This required a second construction of the skeletons, and the validation of that construction is reported at length in Remark 9.4 for a reason: the first two attempts were wrong in a way the output did not reveal. Section 10 records the ring-count series and a conjecture. Section 11 gives the redox bound.

What this article does not do is prove its central bound. Everything substantive is a finite enumeration, which Convention 2.1 admits as axiom-free, and which is checked against Article 62 where the two overlap. But an enumeration is not an explanation, and nothing here explains the bound: a proof must control the capping mechanism, and no argument in this article supplies one. Target 15.1 is therefore the whole of the theorem rather than a gap within it, and Remark 7.8 records what looks like the way in.

1.1 Relation to the experimental programme

The results here are independent of whether any cleavage occurs. Hypothesis 13.1 is carried from Article 83 with its status unchanged — unsupported and not refuted, subject to conditions not available in the open literature — and no theorem of this article asserts it. Were it refuted tomorrow, the theorems would stand and lose their relevance, not their truth. This is deliberate: the journal's subject is the formalism, and a result that waits on a reagent is a result the formalism does not own.

2 Status labels and what this article imports

Convention 2.1 (Status labels; Article 80 [3], Convention 2.1, extended by Article 82 [4])**.** Every assertion in this journal carries one of five labels. **A** finite and axiom-free: the assertion is a statement about a finite structure, and a reader with an independent program obtains the same value. **D** derived under hypotheses named at the point of use. **C** imported from an earlier article of this journal or from the literature, with the locator given. **E** a molecular reading of a structure: an identification of a graph or a formula with a chemical object. **M** measured.

Article 87 is the first article of this corpus to carry no **M** label. It imports no measured quantity and has no counterpart to the membrane tables of Article 83. Of its substantive assertions, all but three are **A** : they are enumerations over graphs on at most 18 vertices, performed in W1–W11 of the verification script. The three exceptions are stated as such where they occur, and two of them are conjectures.

This matters for how the article should be read. Article 83 closed with a scission hypothesis recorded as unsupported and not refuted, and with the observation that the conditions its route requires are not available in the open literature. None of that changes here. What changes is that the obstruction Article 83 reported as a feature of one route is shown to be a property of the skeleton, and therefore a bound that no route can evade.

Convention 2.2 (What is imported)**.** Four integers are imported from Article 62 [1] and carried through Article 83 [2]: the spanning-tree count 1189, the number of chain-forming cut sets 27, the number of distinct C_{18} alkane skeletons 252, and the count of openings admitting a clean ordering, 24 of 27. All four are recomputed here from the skeleton and asserted against the published value; a disagreement would be a defect in one of the two articles and not a tolerance to be widened. An earlier draft of this convention claimed as much while leaving the fourth carried rather than recomputed. Two further integers, the reduction ledger figures 52 and 44 per dimer, are imported from Article 83 section 12 and used only in section 11.

3 The vessel graph and its symmetry

Notation 3.1 (The skeleton as a graph; Article 62 [1], Notation 2.2)**.** Write $\mathsf{X} = (V, E)$ for the chrysene carbon skeleton as an abstract graph: V is the set of 18 carbons, labelled by IUPAC locants 1–12 together with the six ring-fusion locants 4a, 4b, 6a, 10a, 10b, 12a, and E is the set of 21 carbon–carbon bonds. The cyclomatic number is $|E| - |V| + 1 = 4$.
Write $\Phi \subset V$ for the ring-fusion vertices. In this article Φ is *derived* rather than supplied: it is the set of vertices of degree three. The same definition then applies unchanged to every skeleton in section 9, with no hand-written fusion list to go wrong. There are 6 of them.

Write $\Sigma = \{6, 12\}$ for the substituted locants of the 6, 12-disubstituted system of Articles 62 and 83.

Definition 3.2 (Bond classes)**.** Partition E by the number of endpoints lying in Φ. Write $\mathcal{F}$ for the *fusion–fusion* bonds, those with both endpoints in Φ; the mixed class has exactly one; the remaining class has none. The three classes have 5, 8 and 8 members.

Remark 3.3 (Fusion–fusion bonds are not chords)**.** Write C for the *chords* of X: the edges lying in two rings of the parent. There are 3 of them, and $C \subsetneq \mathcal{F}$ properly, the difference being the 2 bonds 4a–4b and 10a–10b. Article 83 named the chords and, at one point in its section 5, counted them where it needed $\mathcal{F}$; the distinction is recorded here because every bound in sections 6–8 is stated in terms of $\mathcal{F}$ and would be false for C. W1 asserts the proper inclusion rather than the cardinalities alone, so that a future edit cannot satisfy the counts while breaking the containment.

Proposition 3.4 (The symmetry of the skeleton)**.** [A] $\mathrm{Aut}(\mathsf{X})$ *has order* 2*. Its nontrivial element* σ *is the involution*

$$\sigma = (1\,7)(2\,8)(3\,9)(4\,10)(4a\;10a)(4b\;10b)(5\,11)(6\,12)(6a\;12a)$$

a product of 9 *transpositions with* 0 *fixed vertices. The edge set falls into* 11 *orbits, of which* 10 *have size two and* 1 *has size one. Moreover* $\sigma(\Sigma) = \Sigma$*.*

Proof. By exhaustive search over vertex bijections respecting adjacency, W2. That σ is an involution and fixes no vertex is checked pointwise. The orbit computation asserts that the orbits partition E, so an orbit miscount cannot pass. □

The last clause of Proposition 3.4 is the one that does work later: because 6 and 12 are interchanged by σ, substituting at both of them *preserves* the symmetry rather than breaking it. The immediate consequence settles a question left open in the discussion around Article 83, section 5.

Corollary 3.5 (The two K-regions are one bond)**.** [A] *The bonds* 11–12 *and* 5–6 *lie in a single orbit of* $\mathrm{Aut}(\mathsf{X})$*, of size* 2*, and they remain in one orbit after substitution at* Σ*.*

Proof. σ carries $11 \mapsto 5$ and $12 \mapsto 6$, hence the one bond to the other; and $\sigma(\Sigma) = \Sigma$ by Proposition 3.4. W2. □

Remark 3.6 (What Corollary 3.5 forbids)**.** There is no regiochemical choice to be made between the two K-regions of a 6, 12-disubstituted chrysene: an instruction to open at 11–12 and an instruction to open at 5–6 name the same experiment and give the same product. Any apparent selectivity between them is statistical, not regiochemical. If a reagent opens one K-region it is as likely to open the other, and the control problem is one of stoichiometry. Note that this is a statement about chemistry and not about cut sets: no chain-forming cut set contains both K-region bonds, so within the combinatorics of this article a doubly opened K-region is not an alternative product but no product at all. This is a statement about the skeleton and is independent of any reaction mechanism. It also vindicates the decision in Article 83, section 5, to resolve the measured attack sites into orbits rather than locants: on a centrosymmetric substrate, locants are not the invariant.

3.1 The quotient by the symmetry

Proposition 3.4 has a consequence for counting that this article must state before it starts counting, because an earlier draft did not. If locants are not the invariant, then neither are counts of locant labellings.

Proposition 3.7 (Orbits of the cut sets)**.** [A] *σ acts on $\mathfrak{K}$ with* 15 *orbits, of which* 3 *are fixed cut sets and* 12 *are pairs. Since $|\mathfrak{K}| = 27$ is odd, at least one fixed cut set is forced. Every invariant tabulated in this article — fusion content, the two clean-ordering counts, the activation index and the substituent pattern — is constant on each orbit, with* 0 *exceptions.*

Proof. W12. The orbit computation asserts that the orbits partition $\mathfrak{K}$; the invariance is asserted across all 15 orbits at once, so a single deviant orbit fails the block. □

Remark 3.8 (Experiments, not labellings)**.** Proposition 3.7 is used twice. As a check it is free and strong: the invariance of five quantities across 15 orbits would be broken by almost any error in the pattern canonicalisation or in the index computation, and it is not. As a statement about counting, it means the figures this article reports — 27 cut sets, 6 realising the target pattern, 12 attaining the activation minimum — correspond to 15, 3 and 7 distinct experiments. Both are given where they occur, and the locant count is retained as the primary one only because it is what the tables index.

4 The cleavage poset

Article 83 introduced sequential cleavage as a procedure and proved one theorem about it. The object that procedure moves

through was left implicit. Naming it is what allows the questions of sections 7 and 8 to be asked at all.

Definition 4.1 (Cut set)**.** A *chain-forming cut set* is a set $\mathsf{K} \subseteq E$ such that $E \setminus \mathsf{K}$ is a Hamiltonian path on V. Write $\mathfrak{K}$ for the collection of these. Necessarily $|\mathsf{K}| = 4$: fewer edges leave a ring, and more disconnect the graph.

Definition 4.2 (The cleavage poset)**.** Fix $\mathsf{K} \in \mathfrak{K}$. The *cleavage poset* $\mathcal{P}(\mathsf{K})$ is the Boolean lattice of subsets of K, ordered by inclusion, where the subset T is read as the *state* in which exactly the bonds of T have been cut: the graph $E \setminus T$ on V. The bottom element is the parent X and the top element is the product chain.
An *ordering* of K is a maximal chain of $\mathcal{P}(\mathsf{K})$ (a linear extension in the sense of [5]), equivalently a sequence $\pi = (e_1, \dots, e_4)$ enumerating K. Write $\Pi(\mathsf{K})$ for the set of orderings, so $|\Pi(\mathsf{K})| = 24$.

Two functions live on this poset. The first classifies a step by the role its bond plays in the substrate *at the moment of cleavage* rather than in the parent; this is the distinction Article 83 drew and it is what makes the criteria below sensitive to the ordering and not merely to the cut set.

Definition 4.3 (The two criteria; Article 83 [2], Theorem 5.15)**.** For a state S let $\mathrm{R}(S)$ denote a smallest set of smallest rings of S. An ordering π is *clean under the weak criterion* w if for each t the bond e_t lies in at most one ring of $\mathrm{R}(S_{t-1})$, where $S_{t-1} = \{e_1, \dots, e_{t-1}\}$. It is *clean under the strict criterion* s if in addition, for each t, not both carbons of e_t lie in two or more rings of $\mathrm{R}(S_{t-1})$. Write $\Pi^{\mathrm{cl}}_{\mathrm{w}}(\mathsf{K})$ and $\Pi^{\mathrm{cl}}_{\mathrm{s}}(\mathsf{K})$ for the two sets, and note $\Pi^{\mathrm{cl}}_{\mathrm{s}} \subseteq \Pi^{\mathrm{cl}}_{\mathrm{w}}$.

Remark 4.4 (On the non-uniqueness of R)**.** A smallest set of smallest rings is not in general unique; see [6] for ring perception in benzenoid systems. What Definition 4.3 uses of it is the number of rings and which edges and vertices lie in two or more of them. For the skeletons enumerated in this article those data are invariant across the choices, and W5 asserts the consequences that the article relies on rather than the intermediate ring sets. A reader implementing Definition 4.3 with a different ring perception should therefore obtain the same integers; if a skeleton were found on which they differ, the criterion and not the computation would need amending.

Definition 4.5 (The activation index)**.** *Throughout, hydrogen counts change only by cleavage.* This is a convention of the poset, not a claim about chemistry: it fixes what the index measures, and section 11 works with a different bookkeeping on structures that are not states of this poset. Let $h_S(v)$ be the number of hydrogens borne by carbon v in state S: in the parent, $h(v) = 0$ for $v \in \Phi \cup \Sigma$ and $h(v) = 1$ otherwise, so that h vanishes on 8 of the 18 carbons; and each cleavage increments h at both of its carbons, since cleaving a bond caps the two carbons it joined. For $\pi \in \Pi(\mathsf{K})$ the *activation index* is

$$\alpha(\pi) \;=\; \#\big\{\, t \;:\; h_{S_{t-1}}(u_t) = h_{S_{t-1}}(w_t) = 0 \,\big\},$$

where $e_t = u_t w_t$. Write $\alpha_{\min}(\mathsf{K}) = \min\{\alpha(\pi) : \pi \in \Pi^{\mathrm{cl}}_{\mathrm{s}}(\mathsf{K})\}$ when $\Pi^{\mathrm{cl}}_{\mathrm{s}}(\mathsf{K}) \neq \emptyset$.

Table 1: Orbits of the edge set of X under $\mathrm{Aut}(\mathsf{X})$, with the bond class of each. Generated by W2.

Size	Bonds	Class
2	1-12a, 6a-7	fh
2	1-2, 7-8	hh
2	2-3, 8-9	hh
2	10-10a, 4-4a	fh
2	10-9, 3-4	hh
2	10a-10b, 4a-4b	ff
2	10a-6a, 12a-4a	ff
2	10b-11, 4b-5	fh
2	11-12, 5-6	hh
2	12-12a, 6-6a	fh
1	10b-4b	ff

Remark 4.6 (Why the index is the right cost)**.** The reaction class Article 83 imports for ring fission installs a diol on the two carbons between which it then cleaves. Where neither carbon bears a hydrogen, that activation cannot be performed, and the step requires a different chemistry. The index counts exactly those steps. Two features of Definition 4.5 are deliberate. It is evaluated at the moment of cleavage, so a step may inherit a hydrogen from an earlier cut that the parent did not supply; and it is a property of the ordering, not of the cut set, so minimising it is a question about chains of $\mathcal{P}(\mathsf{K})$ and not about K alone. Both features are what make $\alpha_{\min}$ smaller than a naive count over $\mathcal{F}$ would suggest.
The index is a combinatorial quantity. That the reaction class it is calibrated against is the chemically operative one is hypothesis H_{crit} of section 13, and it is not established here.

5 The cut sets and their fusion content

Proposition 5.1 (Enumeration)**.** [A] $|\mathfrak{K}| = 27$*; the number of spanning trees of* X *is* 1189*; and the spanning trees realise* 252 *distinct* C_{18} *alkane skeletons up to isomorphism. All three agree with the values published in Article 62 [1].*

Proof. The cut sets by exhaustive search over $\binom{21}{4}$ edge subsets, retaining those whose complement is a Hamiltonian path, W4. The spanning trees twice over, W3: by Kirchhoff's theorem in exact rational arithmetic, with the determinant of the Laplacian minor asserted to be an integer so that a rounding fault cannot pass, and independently by enumeration, with the two counts asserted equal. The skeletons by classifying those trees under a canonical form, so that two trees count once exactly when they are isomorphic. □

Remark 5.2 (Cut sets are not products)**.** The counts measure different things, and the gap between them is where section 8 does its work. A spanning tree need not be a path, and the 1189 of them realise 252 distinct skeletons. The chain-forming cut sets reach only the unbranched one: the 27 of them realise 1 skeleton between them, which W4 asserts rather than assumes.
What distinguishes the cut sets from one another is therefore not the carbon skeleton of the product — that is the same C_{18} chain in every case — but *where on that chain the substituted carbons land*. That is the content of Definition 8.1.

Proposition 5.3 (Fusion content is bounded below)**.** [A] *Every* $\mathsf{K} \in \mathfrak{K}$ *satisfies* $|\mathsf{K} \cap \mathcal{F}| \geq 2$*. The distribution over* $\mathfrak{K}$ *is* 4 *cut sets with exactly two fusion–fusion bonds,* 20 *with three and* 3 *with four, so the content runs from* 2 *to* 4*. In the* 6, 12*-disubstituted system the count* $pc(\mathsf{K})$ *of bonds with no hydrogen on either carbon* in the parent *runs from* 2 *to* 4*.*

Proof. W4, by enumeration over $\mathfrak{K}$. □

Remark 5.4 (What Proposition 5.3 is for)**.** It is tempting to read this as a weak form of the activation bound of section 7: at least two of the four cuts are made between carbons the parent leaves unhydrogenated, so surely at least two steps are obstructed. That reading is wrong, and an earlier draft of this article made it. By Proposition 7.6 the parent count bounds the activation index from *above*, not below, because a carbon unhydrogenated in the parent may be capped by an earlier cleavage. A lower bound on an upper bound constrains nothing.
Proposition 5.3 is therefore not a step towards Theorem 7.1 and is not used in its proof. It is recorded because the fusion content classifies the cut sets in Theorem 6.1, and because the *minimum* of the two quantities turns out to agree on every skeleton computed here, which Remark 7.8 takes up.

6 Clean orderings, and when none exists

Theorem 6.1 (Linearizability)**.** *Let* $\mathsf{K} \in \mathfrak{K}$*.*

(i) [A] *If* $\mathsf{K} \subseteq \mathcal{F}$ *then* $\Pi_s^{\mathrm{cl}}(\mathsf{K}) = \emptyset$*.*

(ii) [A] *For* X*, the converse holds: if* $\mathsf{K} \not\subseteq \mathcal{F}$ *then* $\Pi_s^{\mathrm{cl}}(\mathsf{K}) \neq \emptyset$*.*

Consequently exactly 24 *of the* 27 *cut sets admit a clean ordering, the remaining* 3 *being precisely the* 3 *cut sets contained in* $\mathcal{F}$*.*

Proof. For (i), let $e \in \mathsf{K}$ be whichever bond the ordering takes first. The state before the first step is the parent. In a cata-condensed benzenoid every vertex of degree three lies in two rings, so $e \in \mathcal{F}$ means both carbons of e lie in two or more rings of $\mathrm{R}(\mathsf{X})$, and the strict criterion fails at $t = 1$. Since e was arbitrary in K, it fails for every ordering.
Note that the weak criterion need not fail: a fusion–fusion bond that is not a chord lies in only one ring, which is why (i) is false with w in place of s, and why Remark 3.3 is not a pedantry.
For (ii), by enumeration over the 27 cut sets and all 24 orderings of each, W5. The block asserts the characterisation as an equality of sets, so neither inclusion rests on the other and a counterexample with matching cardinalities could not pass. □

Remark 6.2 (The scope of each clause)**.** Clause (i) holds for any cata-condensed benzenoid. The hypothesis is needed: the proof identifies the degree-three vertices with the vertices lying in two rings, and in a general graph a degree-three vertex may lie in no ring at all, in which case the strict criterion holds and the clause fails. An earlier draft asserted the clause for any skeleton whatever.
Clause (ii) is verified, for X and — by Theorem 9.5 — for each of the other four-ring cata-condensed isomers, and it is open in general. A proof would have to exhibit, for an arbitrary cata-condensed benzenoid and an arbitrary chain-forming cut set not contained in $\mathcal{F}$, an ordering that stays clean to the end; the obvious greedy strategy of taking a non-fusion–fusion bond first is not obviously extensible, because cleaving one bond can promote a second into the shared class.

Proposition 6.3 (How many orderings survive)**.** [A] *Summed over* $\mathfrak{K}$*, the number of strictly clean orderings is* 54*, and of weakly clean orderings* 110*, out of a possible* 27×24*. The per-cut-set strict count ranges from* 0 *to* 8*. Table 2 gives both for each cut set.*

Proof. W5. The two counts are accumulated in one pass, so they cannot disagree about which ordering was examined, and the block asserts that every strictly clean ordering is weakly clean. □

Scholium 6.4. The spread in Table 2 is wide and is not explained here. Several cut sets admit exactly one clean ordering, so that the sequence is forced; one admits 8. Whether the per-cut-set count is a shelling-type invariant of the ring complex, or is computed by some product formula over the fusion pattern, is not addressed. It is the most tractable of the open questions in section 13, because it concerns a known finite table rather than an unbounded family — and because, by Theorem 9.5, whatever explains it must distinguish chrysene from the other four-ring isomers while the cleanly-linearizable count does not.

7 The activation index and its lower bound

Theorem 7.1 (The activation bound)**.** [A] *Over the* 24 *cut sets of* K *admitting a clean ordering,*

$$\min_{\mathsf{K}} \alpha_{\min}(\mathsf{K}) \;=\; 2, \qquad \max_{\mathsf{K}} \alpha_{\min}(\mathsf{K}) \;=\; 3.$$

The minimum is attained by 12 *of them and the maximum by the other* 12*.*

Proof. By enumeration over cut sets and orderings, W6. □

Corollary 7.2 (The obstruction is a property of the skeleton)**.** [A] *Every clean sequential linearization of a* 6, 12*-disubstituted chrysene contains at least* 2 *steps at which neither carbon of the bond being cut bears a hydrogen* in the substrate as it then stands*.*

Remark 7.3 (The qualifier is not decoration)**.** Corollary 7.2 is a statement about states of the poset, not about the parent. Dropping "as it then stands" — as an earlier draft of this corollary did — converts it into a statement about pc, which by Proposition 7.6 runs in the opposite direction and would make the corollary false as a reading of the theorem.

Remark 7.4 (The bound does not depend on which criterion is used)**.** Theorem 7.1 is stated over the cut sets admitting a clean ordering under the strict criterion. Under the weak criterion all 27 cut sets admit one, and the minimum is still 2; the three cut sets that become available are the all-fusion ones of Theorem 6.1, and none of them realises the pattern of section 8, so the excess of Theorem 8.5 is 1 either way. This matters for how much weight the hypothesis H_{crit} of section 13 has to bear. Which criterion is the chemically operative one is open; the bound and the incompatibility do not wait on it.

Remark 7.5 (What this does to Article 83)**.** Article 83 [2], section 5, reported that at two to three of the four steps of its sequence neither carbon bears a hydrogen, and recorded this as an obstruction to the catechol-type activation its cited reaction class uses. Theorem 7.1 sharpens that report in both directions. The lower figure is not an artefact of the particular sequence: it is irreducible, and no choice of cut set or ordering does better. The upper figure is not a defect of the chemistry either: it is what a particular choice of cut set costs, and section 8 shows which choices cost it and why one of them is nevertheless the right one.
Nothing in Article 83 is withdrawn. Its range was correct; what it lacked was the information that the lower end is a floor. A reader could reasonably have inferred that a better sequence might remove the obstruction entirely, and Corollary 7.2 forecloses that.

7.1 The fusion content, and what it does and does not bound

Proposition 7.6 (The parent count bounds the index from above)**.** [A] *For every cut set* K *and every ordering* π *of it,* $\alpha(\pi) \le pc(\mathsf{K})$*, where* $pc(\mathsf{K})$ *counts the bonds of* K *both of whose carbons bear no hydrogen in the parent. The inequality is strict for* 12 *of the* 24 *cut sets admitting a clean ordering.*

Proof. A step contributes to the index only if both its carbons carry no hydrogen at that moment; since cleavage only ever adds hydrogen, such a carbon carried none in the parent. The contributing steps therefore inject into the bonds counted by pc. Strictness is by enumeration, W6, which asserts the inequality as well as counting where it is strict. □

Remark 7.7 (Proposition 5.3 is not a weak form of Theorem 7.1)**.** This correction is recorded because the previous draft had the implication backwards. Proposition 5.3 says $pc(\mathsf{K}) \ge 2$; Proposition 7.6 says pc bounds the index from

Table 2: The 27 chain-forming cut sets of K. Pattern is the substituent pattern of Definition 8.1; |ff| the number of fusion–fusion bonds; Weak and Strict the number of orderings clean under each criterion, of 24; α the minimum activation index over strictly clean orderings. Ordered by α, then pattern. Generated by W5–W7.

Cut set	Pattern	|ff|	*pc*	Weak	Strict	α
1-12a, 10a-6a, 10b-4b, 12a-4a	(2, 11)	3	3	1	1	2
10a-6a, 10b-11, 10b-4b, 12a-4a	(2, 11)	3	3	3	3	2
4b-5, 10a-6a, 10b-4b, 12a-4a	(2, 11)	3	3	3	3	2
6a-7, 10a-6a, 10b-4b, 12a-4a	(2, 11)	3	3	1	1	2
4b-5, 10a-6a, 10b-11, 12a-4a	(2, 17)	2	2	6	6	2
1-12a, 4a-4b, 10a-6a, 10b-4b	(3, 12)	3	3	4	1	2
6a-7, 10a-10b, 10b-4b, 12a-4a	(3, 12)	3	3	4	1	2
10-10a, 10a-6a, 10b-4b, 12a-4a	(4, 13)	3	3	1	1	2
4-4a, 10a-6a, 10b-4b, 12a-4a	(4, 13)	3	3	1	1	2
1-12a, 4a-4b, 6a-7, 10a-10b	(7, 12)	2	2	24	8	2
1-12a, 4a-4b, 10a-10b, 10a-6a	(7, 12)	3	3	12	1	2
4a-4b, 6a-7, 10a-10b, 12a-4a	(7, 12)	3	3	12	1	2
6-6a, 10-10a, 10b-4b, 12a-4a	(1, 10)	2	3	4	4	3
4-4a, 10a-6a, 10b-4b, 12-12a	(1, 10)	2	3	4	4	3
10a-6a, 10b-4b, 11-12, 12a-4a	(1, 10)	3	3	3	3	3
10a-6a, 10b-4b, 12-12a, 12a-4a	(1, 10)	3	4	3	3	3
5-6, 10a-6a, 10b-4b, 12a-4a	(1, 10)	3	3	3	3	3
6-6a, 10a-6a, 10b-4b, 12a-4a	(1, 10)	3	4	3	3	3
1-2, 10a-6a, 10b-4b, 12a-4a	(3, 12)	3	3	1	1	3
7-8, 10a-6a, 10b-4b, 12a-4a	(3, 12)	3	3	1	1	3
2-3, 10a-6a, 10b-4b, 12a-4a	(4, 13)	3	3	1	1	3
8-9, 10a-6a, 10b-4b, 12a-4a	(4, 13)	3	3	1	1	3
10-9, 10a-6a, 10b-4b, 12a-4a	(5, 14)	3	3	1	1	3
3-4, 10a-6a, 10b-4b, 12a-4a	(5, 14)	3	3	1	1	3
10a-10b, 10a-6a, 10b-4b, 12a-4a	(3, 12)	4	4	3	0	—
4a-4b, 10a-6a, 10b-4b, 12a-4a	(3, 12)	4	4	3	0	—
4a-4b, 10a-10b, 10a-6a, 12a-4a	(7, 12)	4	4	6	0	—

above. A lower bound on an upper bound constrains nothing, so Proposition 5.3 implies nothing whatever about $\alpha_{\min}$, in either direction, and Theorem 7.1 is not a sharpening of it. The two are independent facts about the same cut sets, and the gap between them — 12 cut sets where the index falls strictly below *pc* — is the measure of the capping mechanism.

Remark 7.8 (The two minima agree, on every skeleton computed)**.** Despite Remark 7.7, the *minima* of the two quantities coincide: $\min_{\mathsf{K}} |\mathsf{K} \cap \mathcal{F}| = 2$ and $\min_{\mathsf{K}} \alpha_{\min} = 2$. An earlier draft called this a coincidence of this skeleton. It is not: it holds on all 8 skeletons enumerated in section 10, across three ring counts, four chain fusion topologies and one branched skeleton (Table 4). Whatever a coincidence is, it is not something that happens on every available instance. The honest reading is that the data support a strengthening of Conjecture 10.2:

$$\min_{\mathsf{K}} \alpha_{\min} \;=\; \min_{\mathsf{K}} |\mathsf{K} \cap \mathcal{F}| \;=\; k - 2.$$

The right-hand equality is the easier of the two and may well be provable directly from the fusion structure of a catacondensed chain; the left-hand one is Target 15.1. Proving the identity would very likely prove the bound, and this article records it as the most promising available route rather than dismissing it.

Remark 7.9 (What a proof would need)**.** Theorem 7.1 is established by enumeration and is therefore [A] for this skeleton, but it is not proved structurally, and the difference matters for the family statement of section 9. A structural proof must handle the capping mechanism: it is not enough to count fusion–fusion bonds in K, because an earlier cut at a mixed bond can donate a hydrogen to a fusion carbon and spare a later step, which is what Proposition 7.6 records happening in 12 cases. A counting argument would need to bound how many such donations an ordering can arrange, which is a statement about the incidence of K with Φ and not about $|\mathsf{K} \cap \mathcal{F}|$ alone.

Remark 7.10 (Nothing about the bound is currently proved)**.** This should be said plainly, because an earlier draft of this article claimed otherwise. It argued that the first step of an ordering is obstructed whenever both its carbons lie in $\Phi \cup \Sigma$, and concluded that the first-step argument proves $\alpha \geq 1$ where the enumeration gives 2. That conclusion is void. The hypothesis of the first-step argument holds for every bond only when $\mathsf{K} \subseteq \mathcal{F}$, which by Theorem 6.1 is exactly the family Theorem 7.1 excludes; and on the family it does not exclude, 42 of the 54 clean orderings have an unobstructed first step against 12 obstructed. The best bound the argument supplies on the relevant domain is 0. Theorem 7.1 therefore rests on enumeration alone. That is legitimate under Convention 2.1, and the integer is not in doubt. What is in doubt — and what Target 15.1 records — is whether there is any reason for it beyond the enumeration.

8 The product constraint

By Remark 5.2 every chain-forming cut set delivers the same carbon skeleton, an unbranched C_{18} chain. The cut sets are distinguished by where the two substituted carbons land on it. That datum is what connects the combinatorics of this article to the membrane argument of Article 83, because it is what decides which lipid the product is.

Definition 8.1 (The substituent pattern)**.** Let $\mathsf{K} \in \mathfrak{K}$ and let $\gamma = (v_1, \ldots, v_{18})$ be the Hamiltonian path $E \setminus \mathsf{K}$, read in either direction. The *substituent pattern* of K is the pair

$$p(\mathsf{K}) \;=\; \big(\min(i,j),\ \max(i,j)\big), \qquad v_i, v_j \in \Sigma,$$

canonicalised under reversal $i \mapsto 18 + 1 - i$ by taking whichever of the two readings has the smaller first entry. The pattern is therefore an invariant of K and not of a choice of direction along the chain.

Proposition 8.2 (The patterns realised)**.** [A] *Over the* 24 *cut sets admitting a clean ordering, p takes* 7 *distinct values. Exactly* 1 *of them places a substituted carbon at an end of the chain, namely*

$$p^{*} \;=\; (1,\ 10),$$

and p^{*} is realised by 6 *cut sets, which by Proposition 3.7 are* 3 *cut sets up to the symmetry.*

Proof. W7, by enumeration. The patterns are canonicalised before being compared, so a pattern counted twice under opposite readings of the same chain cannot inflate 7. □

Hypothesis 8.3 (The linkage carbon is terminal)**.** H_{term}. [E] Article 62 [1] derives a di-*O*-(octadec-9-en-1-yl) phosphate. The suffix 1-yl places the linkage heteroatom at carbon 1 of an eighteen-carbon chain. The chain delivered by a cut set therefore carries a substituted position at a terminus, and the admissible patterns are those with $p_1 = 1$ or $p_2 = 18$.

Remark 8.4 (The exact extent of the reading)**.** H_{term} is the only [E] assertion on which any theorem of this article depends, and it is worth isolating what it does and does not claim. It claims that the linkage carbon is terminal, which is read off the nomenclature of a published structure. It does *not* claim that the second substituted position, 10, is the distal carbon of the Δ9 alkene, although the arithmetic is consistent with that; Theorem 8.5 needs only the terminus, and the further reading is recorded in section 13 as a non-implication. It does not claim that the substituted carbon of the parent *becomes* the linkage carbon by any particular mechanism. It is worth noting what does follow combinatorially: a terminal substituted position is a carbon that has lost a bond, so all 6 cut sets realising p^{*} cut at a substituted carbon, which W7 asserts. And it does not claim that the Article 62 lipid is reachable: the scission hypothesis H_{scis} of Article 83 remains unsupported and not refuted, and Theorem 8.5 is a conditional statement about which cut sets could deliver that lipid if any of them did.

Theorem 8.5 (Incompatibility of the activation minimum with the required pattern)**.** [A] *Let $\mathsf{K} \in \mathfrak{K}$ admit a clean ordering.*

(i) If $p(\mathsf{K}) = p^{*}$ then $\alpha_{\min}(\mathsf{K}) = 3$.

(ii) If $\alpha_{\min}(\mathsf{K}) = 2$ then $p(\mathsf{K}) \neq p^{*}$.

Hence

$$\min\{\,\alpha_{\min}(\mathsf{K}) : p(\mathsf{K}) = p^{*}\,\} - \min\{\,\alpha_{\min}(\mathsf{K}) : \mathsf{K} \in \mathfrak{K}\,\} \;=\; 1,$$

and the activation minimum of Theorem 7.1 is not attainable by any cut set delivering the pattern H_{term} requires.

Proof. By enumeration, W7. All 6 cut sets realising p^{*} have $\alpha_{\min} = 3$; the block asserts the minimum and maximum of $\alpha_{\min}$ over that family separately, and they are equal, so (i) is an equality and not a bound. Clause (ii) is asserted directly as a statement over the 12 activation-minimal cut sets, rather than inferred from (i), so that the two clauses provide independent checks on the same table. □

Corollary 8.6 (The price of the lipid)**.** [A] [E] *Under* H_{term}*, any clean sequential linearization of a* 6, 12*-disubstituted chrysene that delivers the Article 62 chain contains at least* 3 *activation-obstructed steps, one more than the skeleton's floor.*

Remark 8.7 (The disposition of the recorded sequence)**.** The cleavage sequence recorded for the experimental programme — 11–12, then 12a–4a, then 10b–4b, then 10a–6a — has $|\mathsf{K} \cap \mathcal{F}| = 3$, admits 3 orderings clean under w and 3 under s, of the 24 available, realises the pattern p^*, and has $\alpha_{\min} = 3$. Its stated order — not merely its cut set — is clean under both criteria and attains $\alpha_{\min}$ for that cut set, at 3; W7 replays the recorded order and asserts all three, where an earlier draft asserted them in prose and checked none.
By Theorem 8.5 this is optimal subject to the product constraint. The 12 activation-minimal cut sets — 7 up to symmetry — are not improvements on it: they deliver a different lipid. Stated the other way, the extra obstructed step is the price of the product and not a defect in the choice of sequence, and a reader comparing Theorem 7.1 with Remark 7.5 without Theorem 8.5 in hand would draw the opposite and wrong conclusion.

Scholium 8.8. The shape of Theorem 8.5 is worth noticing independently of its content. Two desiderata on the same finite object — cheapest to activate, and delivering the required product — are optimised by disjoint families of cut sets, and the gap between the two optima is exactly one step. Nothing in the construction of the problem made that inevitable: the two functions $\alpha_{\min}$ and p are defined on the same $\mathfrak{K}$ by unrelated recipes, one over chains of the poset and one over the Hamiltonian path, and they could have agreed. That they do not is a fact about chrysene, and it is the kind of fact a concordance argument in the sense of Article 82 [4] cannot see, because concordance scores a product against measured invariants and is silent about the cost of reaching it.

9 The four-ring isomers

The results so far are about one skeleton. To tell which are facts about chrysene and which about four-ring cata-condensed benzenoids in general, the enumeration is repeated on the other isomers of the same formula. Four of the five are chains and are built by a construction that must itself be checked; the fifth is branched and is supplied directly.

Notation 9.1 (The hexagonal-lattice construction)**.** A cata-condensed benzenoid *chain* is specified by a word of turns: the ring centres walk the hexagonal lattice, each step changing heading by 0 or ± 1 units of sixty degrees. Straight steps give linear fusion and turns give angular fusion; a word of length $k-1$ gives k rings. The four four-ring chain isomers of $C_{18}H_{12}$ are tetracene $(0, 0, 0)$, benz[a]anthracene $(0, 0, 1)$, chrysene $(0, 1, -1)$ and benzo[c]phenanthrene $(0, 1, 1)$. Coinciding ring centres are rejected, so an over-coiled word cannot silently return a peri-condensed graph in place of a cata-condensed one.

Remark 9.2 (The fifth isomer is not a chain)**.** Triphenylene is $C_{18}H_{12}$, has four rings, and is cata-condensed — no carbon lies in three rings — but it is *branched*: a central ring carries three outer rings on alternating bonds, so its ring centres do not form a path and Notation 9.1 cannot build it. Its rings are supplied directly; the ring-fusion vertices are still derived as the degree-three vertices, so no part of the analysis is told by hand what to treat as a fusion carbon.
An earlier draft of this article omitted triphenylene and claimed completeness over the cata-condensed isomers while meaning the chain isomers. Including it costs nothing and settles two of the extremality claims below, in one case against chrysene.

Proposition 9.3 (The construction is validated)**.** [A] *The hexagonal-lattice chrysene is isomorphic as a graph to the IUPAC-labelled* X *of Notation 3.1; the two constructions agree on the spanning-tree count* 1189*; and for each of the* 8 *skeletons built this way the order of* Aut *agrees with the order predicted by the known molecular point group, the molecular plane acting trivially. In particular* $|\,\mathrm{Aut}\,| = 4$ *for naphthalene, anthracene and tetracene,* 2 *for phenanthrene, chrysene and benzo[c]phenanthrene,* 1 *for benz[a]anthracene, and* 12 *for benzene. Hand-supplied triphenylene is checked the same way, at* $|\,\mathrm{Aut}\,| = 6$.

Proof. W11. 3 independent checks, as recorded: isomorphism against the hand-labelled graph, the spanning-tree integer, and the automorphism orders. The last is the check that discriminates between the isomers, since the first two test only the chrysene instance; a word that built the wrong fusion pattern would have to reproduce the right automorphism order by accident.
Benzene appears in the validation set and in no table of the paper, being neither a chain with $k \geq 2$ nor an isomer of $C_{18}H_{12}$; the 7 tabled skeletons are the others. □

Remark 9.4 (Why three checks, and which one fired)**.** This is more validation than a construction of eight small graphs would normally attract, and the reason is recorded because it bears on how the next such enumeration should be done.

The first two attempts at Notation 9.1 were wrong in the same way and the error was invisible in the output: the turn word was taken to have length k rather than $k-1$, so every skeleton was built with one ring too few, and every table of results was internally consistent, plausible, and about the wrong molecules.
What caught it was the chrysene instance failing to reproduce 27 and 24 from Article 62 — an imported corpus integer, not any of the three checks above. An earlier draft of this remark credited the automorphism orders, which is not what happened; the automorphism check was added *afterwards*, because the first failure showed that a construction tested only against quantities it was built to reproduce is not tested at all. Both halves are worth keeping: the imported integer is what fired, and the check that came from outside is what makes the other four isomers believable.

Theorem 9.5 (Invariance across fusion topology)**.** A *For each of the* 5 *four-ring cata-condensed isomers of* $C_{18}H_{12}$*, chains and branched alike:*

(i) exactly 24 *chain-forming cut sets admit a clean ordering;*

(ii) the equivalence of Theorem 6.1 holds, as an equality of sets and not merely of counts, the cut sets admitting no clean ordering being precisely those contained in $\mathcal{F}$*;*

(iii) $\min_{\mathsf{K}} \alpha_{\min}(\mathsf{K}) = 2$.

The total number of cut sets is not invariant: it runs from 24 *to* 27*. Neither is the number of clean orderings, which runs from* 54 *to* 62*. Values are in Table 3.*

Proof. W8, by enumeration on each skeleton, after Proposition 9.3. Clause (i) is asserted as the constancy of the count across the five, so a single deviant isomer fails the block rather than being averaged away. Clause (ii) is asserted per isomer as a set equality; an earlier draft asserted only the cardinalities, which a counterexample with matching counts would have passed. □

Remark 9.6 (Where chrysene is extremal, and where it is not)**.** Chrysene has the fewest clean orderings of the five, 54 against 62, and it is the unique minimiser; that claim survives the inclusion of triphenylene, which gives 60. It offers among the most ways to cut and the fewest ways to sequence a cut.
Two claims an earlier draft made do not survive. Chrysene does not uniquely attain the largest number of cut sets: triphenylene also gives 27, so the maximum is a tie between 2 skeletons. And chrysene does not carry the most fusion–fusion bonds: it has 5, tied among the chains with benzo[c]phenanthrene, but triphenylene has 6, which is the maximum 6 over the five. Both corrections follow from including the isomer the earlier draft left out, and both are recorded rather than quietly amended.
The substance of the remark is unaffected and is clause (i). The count of *cleanly linearizable* cut sets is blind to fusion topology, and blind even to whether the skeleton is a chain; the count of clean *orderings* is not. Whatever invariant explains the first is coarser than whatever explains the second, and Table 3 is the smallest data set on which the two can be told apart.

10 The ring-count series

Proposition 10.1 (The series out to four rings)**.** A *For each of the* 8 *cata-condensed benzenoids with* k *rings listed in Table 4,* $2 \le k \le 4$*,*

$$\min_{\mathsf{K}} \alpha_{\min}(\mathsf{K}) \;=\; \min_{\mathsf{K}} |\mathsf{K} \cap \mathcal{F}| \;=\; k-2.$$

Proof. W9, by enumeration on each of the 8 skeletons. Both equalities are asserted per skeleton, not fitted; the block asserts the agreement of the two minima on all 8 of them. □

Conjecture 10.2 (The ring-count bound)**.** H_{ring}*. For every cata-condensed benzenoid with* $k \ge 2$ *rings,* $\min_{\mathsf{K}} \alpha_{\min}(\mathsf{K}) = k-2$*, independently of the fusion pattern and of whether the skeleton is a chain.*

Remark 10.3 (The standing of Conjecture 10.2)**.** The evidence is 8 skeletons spanning $k = 2, 3, 4$, with all five four-ring isomers agreeing, and it now includes a branched skeleton, which is the only test available outside the chain family. That is enough to make the statement worth recording and not enough to assert it.
Two reasons for caution, and one for encouragement. The fusion pattern is known to matter for neighbouring quantities — by Theorem 9.5 the cut-set count and the clean-ordering count both vary across the four-ring isomers — so the invariance claimed here is not of a piece with everything around it. And at $k = 5$ the helicene words begin to clash on the lattice and the chain family stops being closed under Notation 9.1, so the next case is not merely a larger computation but a question about which skeletons are in the family at all. Against that, the agreement of the two minima recorded in Proposition 10.1 and Remark 7.8 suggests the conjecture may be approachable through the fusion count, which is the more tractable of the two quantities.

Scholium 10.4. The offset has a reading worth stating even though the article cannot prove it is the right one. A catacondensed benzenoid with k rings has cyclomatic number k and so requires k cuts; two of them can be arranged to fall where a hydrogen is available, at terminal rings, which present bonds with hydrogenated carbons. The remaining $k-2$ fall in the interior, where they do not. That is a heuristic and not an argument — it says nothing about whether the two sparing cuts can be taken in an order the clean criterion permits, which is precisely what a proof would have to supply — but it predicts the offset rather than fitting it, and it predicts the fusion-count minimum by the same reasoning, which is consistent with the two agreeing.

11 The oxidation number as a state function

The activation index measures a cost paid step by step, and therefore depends on the ordering. This section records a quantity on the same structures that does not: its value at a state is independent of the route by which the state was reached. The consequence is a bound on redox demand that holds for every mechanism, which is the kind of statement a theoretical article can hand to an experimental programme without waiting on it.

Definition 11.1 (The oxidation-number functional)**.** For a structure S in which each of the 18 skeleton carbons v carries $h_S(v)$ bonds to hydrogen and $o_S(v)$ bonds to oxygen, put

$$\mathrm{ON}(S) \;=\; \sum_{v} \bigl(o_S(v) - h_S(v)\bigr).$$

Proposition 11.2 (Path-independence)**.** ON *is a function of the structure alone. Hence for structures S, S' the net redox demand of passing from one to the other is* $\mathrm{ON}(S') - \mathrm{ON}(S)$*, the same for every route, and in particular the same for every ordering of a cut set and every interleaving of cleavage with reduction.*

Proof. ON is a sum of per-atom quantities evaluated at the structure, with no reference to how the structure was reached; the difference of two such sums is determined by the endpoints. □

Remark 11.3 (The status of Proposition 11.2)**.** This is definitional rather than enumerative, and it carries no status label under Convention 2.1: there is no value for an independent program to reproduce. It is recorded because everything else in this section is a corollary of it, and because the previous draft cited a verification block in its support, which was an error of attribution — the block evaluates ON and does not, because it cannot, establish that ON is a state function.

11.1 The demand fixed by the endpoints

Definition 11.4 (The product chains)**.** [E] Article 62's di-*O*-(octadec-9-en-1-yl) phosphate carries, per chrysene unit, one C_{18} chain: carbon 1 bears the linkage oxygen, carbons 9 and 10 the alkene, carbon 18 the methyl, and the rest are methylene. The ester branch differs at carbon 1 only. Evaluating Definition 11.1 on these gives ON = −34 and ON = −30 respectively, against ON = −8 for the 6, 12-disubstituted core.

Theorem 11.5 (The demand is fixed, and recovers the Article 83 ledger)**.** [D] [C] *Under Definition 11.1, reaching the Article 62 ether chain from the substrate requires a net reduction of* 26 *equivalents per chrysene unit and* 52 *per* 6, 12*-dimer; the ester branch requires* 22 *and* 44*. By Proposition 11.2 these are independent of mechanism, of the cut set, and of the order of operations.*
Article 83, section 12, reports a reduction ledger of 52 *equivalents per dimer on the ether branch and* 44 *on the ester branch, counted along a route. The two agree exactly.*

Proof. Evaluation of Definition 11.1 at the three structures, W10; the substrate is derived from the skeleton rather than written out, and the agreement with Article 83 is asserted rather than observed. □

Remark 11.6 (What the agreement is worth)**.** Article 83 obtained 52 and 44 by counting reductions along a proposed route. Theorem 11.5 obtains the same integers from the two endpoint structures alone, with no route in evidence. That is a check on Article 83 rather than a new result — had the numbers disagreed, one of the two articles would have been wrong — and it upgrades the ledger from a property of a route to a property of the problem.

Corollary 11.7 (A mechanism-independent floor)**.** [D] *No route from the* 6, 12*-disubstituted core to the Article 62 ether chain requires fewer than* 26 *reducing equivalents per unit. A route claiming less is in arithmetic error, not in possession of a better mechanism.*

Remark 11.8 (What path-independence does not buy)**.** Corollary 11.7 bounds a total, not a path. It says nothing about rate, about feasibility, or about the availability of a

Table 3: The 5 four-ring cata-condensed isomers of $C_{18}H_{12}$. "Clean" counts cut sets admitting a clean ordering; "Clean ord." counts clean orderings summed over cut sets. The 4 unmarked rows are chains, built by Notation 9.1; † marks the branched isomer, whose rings are supplied directly. Generated by W8.

Isomer	| Aut |	Cut sets	Clean	Clean ord.	|ff|	min |ff|	$\alpha_{\min}$
tetracene	4	24	24	62	3	2	2
benz[a]anthracene	1	25	24	62	4	2	2
chrysene	2	27	24	54	5	2	2
benzo[c]phenanthrene	2	26	24	62	5	2	2
triphenylene †	6	27	24	60	6	2	2

Table 4: The ring-count series. $\alpha_{\min}$ is the minimum activation index over all cut sets and clean orderings; it equals min |ff|, and both equal $k-2$, throughout. † marks the branched skeleton. Generated by W9.

Skeleton	Rings	C	Bonds	Cut sets	Clean	min |ff|	$\alpha_{\min}$
naphthalene	2	10	11	12	12	0	0
anthracene	3	14	16	18	18	1	1
phenanthrene	3	14	16	19	18	1	1
tetracene	4	18	21	24	24	2	2
benz[a]anthracene	4	18	21	25	24	2	2
chrysene	4	18	21	27	24	2	2
benzo[c]phenanthrene	4	18	21	26	24	2	2
triphenylene †	4	18	21	27	24	2	2

reductant at a given potential, and a demand that a ledger can meet in aggregate may still be unmeetable step by step. It is also silent on the *oxidant* side: a route that climbs before it descends spends on both, and Proposition 11.10 is where that shows up.

11.2 Two routes to the same product

Definition 11.9 (The oxidative and reductive routes)**.** Fix a cut set K. On the *oxidative* route I each bond of K is cleaved while the skeleton is still aromatic, so every carbon K severs takes a carbonyl and nothing else changes. On the *reductive* route II the skeleton is first reduced so that every carbon *not* severed by K is sp^3, which presents each bond of K as an isolated alkene, and those alkenes are then cleaved.
Both states are derived from K. Neither is the product of Definition 11.4; both are intermediates on the way to it.

Proposition 11.10 (The excursion)**.** D *Let* K *admit a clean ordering. Then the oxidative intermediate lies* above *the substrate by* 14 *or* 16 *equivalents, according to* K*, and the reduced precursor lies* below *it, between the substrate and the product. Define the redox traffic of a route as the total movement in* ON *along it, counting an excursion above the product twice. Then*

$$\mathit{traffic}(\mathrm{I}) \in \{54, 58\}, \qquad \mathit{traffic}(\mathrm{II}) = 26,$$

a ratio of 2.08 *to* 2.23*. The net demand of the two is identical, by Proposition 11.2; only the traffic differs.*

Proof. W10, by evaluation over the 24 cut sets admitting a clean ordering. That the reduced precursor lies between substrate and product — so that II never climbs — is asserted rather than inferred. □

Remark 11.11 (Why the figures depend on the cut set)**.** A cut set with four pairwise disjoint bonds severs eight distinct carbons; one in which a carbon is cut on both sides severs seven. The number of carbonyls installed differs accordingly, and so does ON at the intermediate. Of the 27 cut sets, twelve sever eight carbons, twelve sever seven, and 3 sever six — and those 3 are exactly the cut sets whose severed set is the six ring-fusion carbons, which by Theorem 6.1 are exactly the cut sets admitting no clean ordering. The section therefore has to be stated per cut set; there is no single pair of numbers for it.

Remark 11.12 (Withdrawal of the redox-neutrality claim)**.** The previous draft of this section asserted that the reductive route is redox-neutral on the skeleton, passing from ON = −8 to −20 and back to −8. That is withdrawn. The computation rested on four hand-written per-carbon state vectors that installed six carbonyls where four cleavages

sever eight carbon ends, and the apparent neutrality was the arithmetic coincidence of twelve added hydrogens matching the twelve carbon–oxygen bonds of six carbonyls. The vectors were realised by exactly the 3 cut sets of Remark 11.11, which this article elsewhere proves are not cleanly linearizable: the section computed on the one case the rest of the paper excludes.

Recorded rather than absorbed, per the correction convention of Article 82 [4]. The corrected statement is Proposition 11.10, which makes a weaker claim about the routes and a stronger one about the problem: the net demand is the same for both routes, because ON is a state function, and what separates them is traffic.

Remark 11.13 (The activation index does not reach these states)**.** The previous draft also asserted that the reductive route resolves the activation obstruction, on the ground that a carbon made sp^3 bears hydrogen. That is withdrawn too, and so is its negation, which a review of this article proposed in its place.

The index of Definition 4.5 is defined on the cleavage poset of the *aromatic* skeleton, where the only thing that changes a hydrogen count is a cleavage. The reduced precursor of Definition 11.9 is not a state of that poset: reaching it changes hydrogen counts by reduction, which the poset does not model. Evaluating α there is a category error, and the error runs in both directions — one may neither claim that the reduction installs the hydrogens the obstruction wants, since it installs them precisely at the carbons that are not being cut, nor that the route is therefore maximally obstructed, since the index is not defined on its states at all. What can be said is narrower and is said in section 13: whether the index is the operative cost is hypothesis H_{crit}, and whether a reduced substrate changes which chemistry performs a step is outside this article.

Remark 11.14 (The direction of the biological evidence)**.** Article 83 [2], section 13, cited the ring-reduction intermediates of the anaerobic naphthalene pathway [7, 8] — the dihydro, tetrahydro and hexahydro thioesters — as evidence that the biological chemistry runs opposite to the direction the construct requires.

Proposition 11.10 bears on that reading without settling it. Reduction before cleavage is not an overhead to be paid in addition to the demand of Theorem 11.5: by path-independence it is part of that demand, and a route taking it monotonically spends less total traffic than one that climbs first. To that extent the biological order of operations is the economical one.

Three cautions limit the amendment, and the previous draft stated only the first two. The biological pathway requires a thioester handle to make its rings reducible, which the chrysene skeleton does not have. Its ring cleavage is hydrolytic rather than oxidative, so its endpoint is not the endpoint of Definition 11.4 and Theorem 11.5 does not transfer to it unchanged. And traffic is not a cost function that any experiment has been shown to minimise; it is an accounting quantity, and calling the monotone route economical is a statement about arithmetic, not about chemistry.

12 Consolidated register

Table 7 indexes the 13 verification blocks. The script emits 108 values and 7 tables; every number printed in this article is one of those values, and check C1 of Article 82 [4] is performed by block W13 against the paper sources in both directions, so a value emitted and not used, or used and not emitted, fails the run. An earlier draft asserted that enforcement without implementing it anywhere.

The substantive results, with their status:

- A | Aut(X)| = 2; the two K-region bonds form one orbit; Σ is σ-stable; the 27 cut sets fall into 15 orbits on which every tabulated invariant is constant (Propositions 3.4 and 3.7, Corollary 3.5).
- A $|\mathfrak{K}| = 27$, spanning trees 1189, alkane skeletons 252, all agreeing with Article 62; the cut sets realise 1 of those skeletons between them (Proposition 5.1).
- A $\mathsf{K} \subseteq \mathcal{F} \Rightarrow \Pi_{\mathrm{s}}^{\mathrm{cl}}(\mathsf{K}) = \emptyset$, proved for cata-condensed benzenoids; the converse verified for X and the four other four-ring isomers, as a set equality (Theorems 6.1 and 9.5).
- A $\min_{\mathsf{K}} \alpha_{\min} = 2$, attained, and unchanged under the weak criterion (Theorem 7.1, Remark 7.4); the obstruction is a property of the skeleton (Corollary 7.2).
- A pc bounds $\alpha_{\min}$ from above, strictly in 12 cases (Proposition 7.6); the two *minima* agree on all 8 skeletons computed (Remark 7.8).
- A Exactly 1 substituent pattern is terminal, namely $p^* = (1, 10)$ (Proposition 8.2).
- A Every cut set realising p^* has $\alpha_{\min} = 3$, and no activation-minimal cut set realises p^* (Theorem 8.5).
- A All 5 four-ring cata-condensed isomers, branched included, have 24 cleanly linearizable cut sets and $\alpha_{\min}$-minimum 2; chrysene uniquely minimises the clean-ordering count (Theorem 9.5).

Table 5: Oxidation number along the two routes, per chrysene unit. ON is a state function, so the demand between any two rows is fixed; the intermediate rows depend on the cut set, which is why they carry a range rather than a value. Generated by W10.

State	ON	Relation to the substrate
6,12-disubstituted chrysene core	−8	—
oxidative intermediate	—	above by 14 or 16, by cut set
reduced precursor	—	below by 10 or 11, by cut set
Article 62 ether chain	−34	below by 26; 52 per dimer
Article 62 ester chain	−30	below by 22; 44 per dimer

- D The demand from the substrate to the Article 62 ether chain is 26 equivalents per unit, 52 per dimer, independently of mechanism, recovering the Article 83 ledger (Theorem 11.5).

13 Hypotheses and non-implications

Hypothesis 13.1 (Carried from Article 83)**.** H_{scis}. D The 6, 12-disubstituted chrysene undergoes cleavage at the loci of a chain-forming cut set, without loss of carbon, in a clean sequential order. Article 83 records this as unsupported and not refuted, subject to conditions not available in the open literature [9]. Its status is unchanged here. *Every theorem of this article is conditional on nothing but the skeleton; none of them asserts H_{scis}, and none would be falsified by its refutation.* What would be lost on refutation is the relevance of the results, not their truth.

Hypothesis 13.2 (The criterion is the chemical one)**.** H_{crit}. D The strict criterion s of Definition 4.3 is the one that governs which steps a catechol-type activation can perform, and the activation index of Definition 4.5 is therefore the operative cost. Article 83, section 5, raised this question and did not settle it; it is not settled here.
Its weight is smaller than it was. By Remark 7.4 the bound of Theorem 7.1 and the excess of Theorem 8.5 are the same under either criterion, so the article's conclusions do not wait on it. What does wait on it is the clean-ordering counts of Table 2, and the reading of the index as a chemical cost rather than a combinatorial one.

Hypothesis 8.3 (H_{term}) and Conjecture 10.2 (H_{ring}) complete the list. Table 6 collects all 4.

Non-implications. The following are *not* claimed, and a reader who takes any of them from this article has read more than is written.

(N1) *That chain position* 10 *of the product is the distal carbon of the* Δ9 *alkene.* The arithmetic is consistent with it and Remark 8.4 declines to assert it. Theorem 8.5 uses only the terminus.

(N2) *That the activation-minimal cut sets are better experimental targets.* They are cheaper to activate and they deliver a different lipid; the two properties are incompatible by Theorem 8.5.

(N3) *That the activation index bounds any rate, yield or feasibility.* It counts steps of one kind. A step it does not count may still fail.

(N4) *That Proposition 5.3 supports Theorem 7.1.* It does not, in either direction; Remark 5.4 and Proposition 7.6 say why.

(N5) *That anything about Theorem 7.1 is proved.* Remark 7.10 withdraws the claim an earlier draft made, and nothing replaces it.

(N6) *That Conjecture 10.2 is established.* It is checked on 8 skeletons to $k = 4$, and Remark 10.3 gives two reasons to withhold assertion.

(N7) *That* ON *bounds the reductant a route needs step by step.* Corollary 11.7 bounds a total; Remark 11.8 separates the two.

(N8) *That either route of Definition 11.9 is reachable, or that redox traffic is a cost any experiment minimises.* Section 11 computes an accounting quantity. Remark 11.14 says what that does and does not license.

(N9) *That the activation index says anything about the reduced structures of section 11.* It is not defined on them; Remark 11.13 withdraws both the claim an earlier draft made and the opposite claim proposed in its place.

14 Precedence

Ruling 14.1 (Article 83, section 5: strengthened, not corrected)**.** Article 83 reported that two to three of the four steps of its sequence cut bonds with no hydrogen on either carbon. That range is correct and is not withdrawn. Theorem 7.1 adds that the lower end is a floor over all cut sets and all clean orderings, and Theorem 8.5 identifies the upper end as the cost of the required product. The report stands; what

is added is that neither figure is an artefact of the route.

Ruling 14.2 (Article 83, section 12: confirmed from the endpoints)**.** Article 83's reduction ledger of 52 and 44 equivalents per dimer was obtained by counting along a proposed route. Theorem 11.5 obtains the same integers from the endpoint structures alone, by path-independence. The ledger is confirmed and is upgraded from a property of a route to a property of the problem. No amendment to Article 83 follows.

Ruling 14.3 (Article 83, section 13: no amendment)**.** An earlier draft of this article withdrew Article 83's reading of the anaerobic naphthalene intermediates and replaced it with the claim that ring reduction is the activating step. That withdrawal is itself withdrawn. The claim rested on evaluating the activation index at structures on which it is not defined (Remark 11.13), and the supporting arithmetic was the redox-neutrality result that Remark 11.12 retracts. What survives is weaker and is stated in Remark 11.14: a monotone route spends less redox traffic than one that climbs, which is an observation about accounting and not a reinterpretation of the biological evidence. Article 83 section 13 therefore stands unamended, and this ruling exists to record that a proposed amendment was raised and rejected rather than to leave the matter silent.

Ruling 14.4 (The recorded sequence)**.** The cut set recorded for the experimental programme realises p^{*} and attains $\alpha_{\min}$ for that cut set, and the recorded *ordering* is clean under both criteria and attains that index, which W7 now checks rather than assuming. By Theorem 8.5 the choice is optimal subject to the product constraint, and the 12 activation-minimal cut sets are not alternatives to it. No change to the recorded sequence follows from this article.

Ruling 14.5 (Article 72, Target 11.11: not addressable as stated)**.** Recorded for completeness. Article 72's [10] Target 11.11 asks that E^{*} be matched against a membrane modulus. Article 83 established that E^{*} is a duplex bending tolerance and not a membrane modulus, so the target is not addressable as written and requires restatement or withdrawal before any article can discharge it. Article 84 does not restate it, and Target 11.8, the curvature floor, likewise remains open.

15 Obligations

Target 15.1 (A structural proof of the activation bound)**.** Prove Theorem 7.1 without enumeration, and deduce Conjecture 10.2. By Remark 7.9 the obstacle is the capping mechanism: a bound must control how many fusion carbons an ordering can hydrogenate in advance of the steps that need them, which is a statement about the incidence of K with Φ and not about $|\mathsf{K} \cap \mathcal{F}|$ alone. Nothing is currently proved, so the target is the whole of the theorem and not a gap within it. The most promising route on the evidence is through the identity of Remark 7.8.

Target 15.2 (The identity of the two minima)**.** Prove or refute $\min_{\mathsf{K}} \alpha_{\min} = \min_{\mathsf{K}} |\mathsf{K} \cap \mathcal{F}|$ for cata-condensed benzenoids. It holds on all 8 skeletons computed here. The right-hand side is a statement about the fusion structure alone, with no reference to orderings, and is for that reason the more tractable of the two; a proof of the identity would reduce Target 15.1 to it.

Target 15.3 (The converse of Theorem 6.1)**.** Prove or refute, for an arbitrary cata-condensed benzenoid, that a chain-forming cut set not contained in $\mathcal{F}$ admits a strictly clean ordering. Remark 6.2 notes why the greedy strategy does not obviously extend.

Target 15.4 (The clean-ordering count)**.** Account for the per-cut-set clean-ordering counts of Table 2, which range from 0 to 8, and for the fact that chrysene uniquely minimises the total at 54 while the cleanly-linearizable count is constant at 24 across all 5 isomers. The invariant sought here is finer than whatever makes that count constant.

Target 15.5 (The five-ring family)**.** Settle which five-ring cata-condensed benzenoids are admissible, the helicene words beginning to clash on the lattice at $k = 5$, and test Conjecture 10.2 on them. The branched members matter as much as the chains, triphenylene having shown that the conjecture does not depend on being a chain.

Target 15.6 (The authoritative bibliography)**.** Bibliography entries for articles of this corpus were reconstructed from titles for Article 83 and are carried here. They should be checked against the authoritative file before the volume is closed. Recorded as an obligation rather than silently repaired.

16 Conclusion

Article 83 computed a membrane from a cleavage family and scored it against measured invariants. It left an obstruction in its section 5 — that at two to three of four steps the activation its reaction class requires cannot be performed — as a reported feature of a particular route. This article names the object that route moves through, the cleavage poset of the skeleton, and shows that the obstruction belongs to the skeleton rather than to the route: the index is at least 2 for every cut set and every clean ordering, under either criterion, and the bound is attained.

The result that was not anticipated is the incompatibility. The requirement that the linkage carbon be terminal, which is what the Article 62 lipid means by 1-yl, selects a single substituent pattern out of the 7 available, and every cut set realising it carries index 3 rather than 2. The lipid costs one obstructed step more than the skeleton's floor, and the sequence recorded for the experimental programme is optimal given that cost rather than improvable by a better choice. Two functions defined on the same finite set by unrelated recipes turn out to be optimised by disjoint families, and the gap is exactly 1.

What the article does not do is prove the bound. Everything substantive is a finite enumeration, legitimate under Convention 2.1 and checked against Article 62 where the two overlap, but an enumeration is not an explanation. An earlier draft claimed a first-step argument established part of the bound; it does not, on the domain where the bound lives, and Remark 7.10 withdraws the claim. Target 15.1 is accordingly the whole of the theorem rather than a gap within it, and Target 15.2 is the most promising way in.

Three methodological points are worth recording, because each cost something.

A construction validated only against the quantities it was built to reproduce is not validated. The isomer comparison was twice computed on skeletons with one ring too few, and the output was internally consistent both times; what caught it was an imported corpus integer, and what makes the other isomers believable is a check from outside (Remark 9.4).

A stated convention is not an implemented one. An earlier draft of section 12 claimed that check C1 was enforced in both directions. It was not implemented anywhere, and the claim was true of that build only by accident. It is implemented now, and it fired on the first run against the rebuilt section 11.

And a quantity optimised in isolation is not optimised. The first reading of this enumeration concluded that the recorded cut set was one step worse than necessary and that twelve better choices existed. That reading is inverted by Theorem 8.5, which is now the paper's main result: the twelve deliver a different product. The error came of optimising one of two functions on the same finite set without asking what the other did, and it is the same error, in a different register, as computing section 11 on the one family that section 6 excludes.

Table 6: The 4 hypotheses. Only H_{term} is used by a theorem; H_{scis} is carried, H_{crit} is open but the bound does not depend on it, H_{ring} is a conjecture. Emitted with the tables, outside any block.

Name	Status	Assertion	Standing
H_{scis}	D	cleavage at the loci of a cut set, without carbon loss, in clean order	carried from Article 83; status unchanged
H_{term}	E	the linkage carbon of the Article 62 chain is terminal	introduced here; used by the incompatibility theorem only
H_{crit}	D	the strict criterion is the one the activation chemistry obeys	raised in Article 83; open, but the bound is independent of it
H_{ring}	D	the activation minimum is $k-2$ for every cata-condensed benzenoid	conjecture; checked on 8 skeletons

A Reproduction

The verification script is standard-library Python, writes relative to its own location, asserts rather than prints, and exits non-zero on any failure. It emits 108 values and 7 tables across 13 blocks. Graph primitives are held in a separate module so that each can be exercised on more than one skeleton; nothing in that module knows which molecule it is applied to, and the ring-fusion vertices are derived as the degree-three vertices rather than supplied by hand.

Four features are worth naming for a reader reproducing the work. Macro names are asserted to be letters only, because a digit in a control sequence truncates it silently and produces a build failure far from its cause. Data labels are escaped at emission, because a per cent sign in a label comments out the remainder of its table row and passes every other check. The block index of Table 7 is generated from the script's own source and asserted to agree with it, so a block added without being indexed fails the run. And check C1 is performed in `W13` against the paper sources, comment tails stripped so that a macro named only in a comment does not count as used; the check runs when the sources sit beside the script, as they do in the verification archive, and is skipped when they do not.

B What the enumeration does not establish

The enumeration establishes statements about X and the eight other skeletons named. It does not establish that any bond is cleaved, that any reagent performs any step, that the orderings

Table 7: Index of the 13 verification blocks. Generated from the script and checked against it.

Block	Content
W1	the vessel graph: order, size, bond classes, chords
W2	the automorphism group and the orbit of the K-region
W3	spanning trees and the alkane skeletons they reach
W4	chain-forming cut sets and their fusion content
W5	clean orderings, and when none exists
W6	the activation index
W7	the substituent pattern of the product
W8	the four-ring isomers, chain and branched
W9	the ring-count series, and the fusion-content identity
W10	the oxidation number as a state function
W11	validation of the hexagonal-lattice construction
W12	the quotient by the automorphism group
W13	check C1, against the paper sources, in both directions

called clean are chemically preferred, or that the index of Definition 4.5 is the operative cost — that last being Hypothesis 13.2, which is open, though by Remark 7.4 the bound and the excess are the same under either criterion.

Three further limits are worth stating separately, because an earlier draft of this article overstepped each of them. It does not *prove* Theorem 7.1: the theorem rests on enumeration and nothing here explains it. It does not establish anything about the reduced structures of section 11 beyond their oxidation numbers — the activation index is not defined on them, in either direction. And the redox traffic of Proposition 11.10 is an accounting quantity, not a cost any experiment has been shown to minimise.

The non-implications of section 13 list the specific readings the article declines.

References

[1] Charles D. Schaper. The Enclosure via the Encoded Chrysene Cluster: Integrated Synthesis of Nucleic Acids and Phospholipids, and the Orientational Encoding of the Membrane. *Annals of the Chrysene Formalism*, 1(3):1279–1320, 2026. Article 62. DOI: https://doi.org/10.68366/24m3wx88.

[2] Charles D. Schaper. The Transformed Product: Membrane Invariants Measured against the Open Literature, and the Lipid the Patent Route Actually Makes. *Annals of the Chrysene Formalism*, 1(4):1675–1702, 2026. Article 83. DOI: https://doi.org/10.68366/1aey1m29.

[3] Charles D. Schaper. The Completeness Condition: Realisation of the Twelve-Axiom Framework at a Site of the Interior Chrysene Lattice, and the Genome Length It Requires. *Annals of the Chrysene Formalism*, 1(4):1639–1651, 2026. Article 80. DOI: https://doi.org/10.68366/0a19r769.

[4] Charles D. Schaper. The Partition Concordance: Arm Additivity Measured against the Open Literature, and the Reassignment of Purity to the Structural Filters. *Annals of the Chrysene Formalism*, 1(4):1662–1674, 2026. Article 82. DOI: https://doi.org/10.68366/qxw27909.

[5] R. P. Stanley. *Enumerative Combinatorics, Volume 1*. Cambridge University Press, 2 edition, 2012.

[6] I. Gutman and S. J. Cyvin. *Introduction to the Theory of Benzenoid Hydrocarbons*. Springer-Verlag, Berlin, 1989.

[7] P. Weyrauch, I. Heker, A. V. Zaytsev, C. A. von Hagen, M. E. Arnold, B. T. Golding, and R. U. Meckenstock. Conversion of Cis-2-Carboxycyclohexylacetyl-CoA in the Downstream Carboxylic Acid Degradation Pathway of the Anaerobic Naphthalene Degradation. *Applied and Environmental Microbiology*, 86(19):e00996–20, 2020. DOI: https://doi.org/10.1128/AEM.00996-20.

[8] R. U. Meckenstock, E. Annweiler, W. Michaelis, H. H. Richnow, and B. Schink. Anaerobic naphthalene degradation by a sulfate-reducing enrichment culture. *Applied and Environmental Microbiology*, 66(7):2743–2747, 2000. DOI: https://doi.org/10.1128/AEM.66.7.2743-2747.2000.

[9] Charles D. Schaper. Encoded Design Integrated Synthesis of Nucleic Acids, and Phospholipids, and Related Pharmaceutical Products. United States Patent No. 12,195,423 B1, 2025. Figure 16(b), Figure 9(a)–(c), Figure 17 and col. 57 are the loci used here.

[10] Charles D. Schaper. Cycle Integration: Copy Number, the Closure Vesicle, and the Band of the Genome. *Annals of the Chrysene Formalism*, 1(3):1472–1483, 2026. Article 72. DOI: https://doi.org/10.68366/7fdnjs23.