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The Enclosure via the Encoded Chrysene Cluster

Integrated Synthesis of Nucleic Acids and Phospholipids, and the Orientational Encoding of the Membrane

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Abstract. The encoding of the corpus operates on a complex of two units: a 6,12-disubstituted chrysene paired with a 3,6,9,12-tetrasubstituted one. The tetrasubstituted unit becomes a nucleobase; the disubstituted unit is the template on which it is shaped, is not consumed, and remains tethered to the base it templated, holding still the two binary orientational data — its alignment to its partner, and its orientation in the cluster's common frame — whose pair indexes base four and constitutes the encoding. A tethered unit is therefore not a label on a sequence but a carrier of it. This paper asks what becomes of those carriers, and of the units of the same family never recruited into a complex. The two questions have one answer: the unrecruited remainder makes a membrane, and the carriers migrate into it, so that an enclosed reaction environment arises from the material of the encoding itself.

Scission is finite and enumerated in full. Four are attachment-admissible; one places its tails in the lamellar range, the selection being by tail length and not by topology. Eliminating rather than reducing the ether at the free substituted position fixes the retained unsaturation at Δ9, and the product is a di-*O*-(octadec-9-enyl) phosphate, each of whose defining features the enumeration fixed before any comparand was consulted. The minority doubly bridged dimer yields a macrocyclic bolaamphiphile instead. Enclosure is a parity condition: the leaflet map is a $\mathbb{Z}/2$-valued function on the anchor set, and the strand is enclosed exactly when it is constant, crossing the core once at each sign change. The condition is not metric, and since a crossing would carry a charged backbone through an acyl core at a cost of order $10^2\, k_B T$, the constant case is the one with a route: enclosure reduces to a single bit fixed at closure.

The passage of the encoding into the membrane is posed as a question about a map. The source carries two bits per anchor. One is the pair type, written into the molecule as a tether and a cap by the same event that recorded it, and carried unconditionally. The other is frame-relative, and a closed membrane supplies the frame: its normal is globally defined, so the face a unit presents is one question at every anchor—the condition under which the anchors encode collectively rather than severally. Whether a unit is free to record in that frame is a premise about a nine-atom arm, and it separates two cases: the map injective at two bits per anchor, or the face slaved to the pair type, with fibres of size 2^m and the polarity of every base pair lost. That premise competes with the premise on which the anchoring has a subject at all, both being demands on the same arm. The anchors' ordering is carried by the strand's covalent backbone and costs no premise; a second channel, filtered by helical phase, resolves e bits for e anchors in phase and adds redundancy rather than resolution. Closure requires an unrecruited pool of order 10^2 vessels per encoded vessel under a stipulated bending tolerance, and the requirement does not grow with the sequence enclosed. Because the strand is anchored rather than free, the operative condition is a curvature and not a volume.

Keywords: Chrysene Formalism; encoded chrysene cluster; integrated synthesis; nucleic acids; phospholipids; orientational encoding

1 Introduction

The corpus carries an encoded cluster of π-stacked chrysene units through a transformation to an intercalated nucleic acid tethered to its paired unit. The residue account takes that object and asks what becomes of the tethered arm, answering with an amino-acid residue at a transannular centre and a parity condition governing the hand of an assembly. The present paper takes the same object at the same point and asks a different question of it.

What the encoding operates on is a complex of two units, and the distinction between them is the whole of what follows. The 3,6,9,12-tetrasubstituted unit is the one transformed into a nucleobase. The 6,12-disubstituted unit is the template on which that transformation is shaped; it is not consumed; and it

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remains tethered to the product it templated. Its orientation at the moment of templating — aligned or unaligned to its partner, and oriented one way or the other in the frame common to the cluster — is what determined which base was made. Those two binary data are the encoding, and the unit still holds them.

Two things the corpus has not asked, and they are connected. The first concerns what the tether is for. A tethered unit is not a tag fastened to a nucleic acid after the fact; it is the object whose orientation decided the base, still attached to it. The second concerns the units of the same family that were never recruited into a complex. An assembly draws some of its pool into complexes and leaves the rest, and the corpus has treated the remainder as remainder.

The connection is that the remainder and the carrier are the same molecule in two roles. An unrecruited 6,12-disubstituted dimer, cut along the loci at which the corpus already records scission, is an amphiphile; a surface of such amphiphiles is a bilayer; and a tethered unit of the same family, unscissioned, belongs in that surface because the surface is made of its own kind. What the tether is for, on this reading, is to carry an encoding into a membrane built from the units that did not encode.

1.1 What this paper addresses

Three questions, in the order the paper takes them.

Whether the unrecruited pool can close a surface at all, which is a question about cut sets and a carbon budget and is answered finitely in Sections 5 and 6.

Whether an anchored strand is inside that surface or outside it, which is a question about a two-valued function on a finite set and is answered in Section 8, subject to a premise supplied in Section 7 about how the tethered unit sits.

And how much of the encoding survives the passage into the surface, which is answered in Section 9 as a channel problem: a source of two bits per anchor, a surface state of at most two, and a premise about the flexibility of a tether separating the lossless case from the one that keeps the pair types and loses the polarities.

Section 10 asks what the setting must supply for any of this to occur, and returns a ratio rather than a count.

1.2 What is established here, by kind

Recovered. The complex of a 6,12-disubstituted unit paired with a 3,6,9,12-tetrasubstituted one, the templating role of the first and its retention on the tether; the two tethers with their caps and the orientational datum they carry; the vessel graph and its locant registry; the reachability convention. Imported unamended at Sections 2 and 4.

Proved here. The scission classification and the position of the retained unsaturation (Theorems 5.10, 5.20); the encapsulation condition (Theorem 8.3); the orientation relation $\sigma = \omega + \lambda$ and the congruence criterion it yields (Theorem 9.23, Corollary 9.25); the stoichiometric bound on closure (Theorem 10.5).

Found. That the edge at which the elimination fixes the tail's unsaturation is the edge the residue account severs (Remark 5.22); that the bilayer normal supplies globally the common frame the cluster's stack supplied, and is the only datum of a fluid surface that does (Proposition 9.20); that the passage is injective or two-to-one at each anchor according to a single premise about the flexibility of a tether (Theorem 9.24); and that the two conformational premises of Sections 7 and 9 make competing demands on the same arm, so that their conjunction is stronger than either (Remark 7.12).

Proposed, and not addressed. That injectivity is the condition without which no decoding of the surface could occur, that the architecture meets it under one premise, and that the tethering complex is the covalent structure along which a decoding would run (Remark 9.28, Target 14.11). Signalling and modulation between an enclosure and the sequence it encloses are a subject for later work.

Computed here. The cut-set enumeration and the four routes; the reduction ledger and the product formula; the skeleton geometry, and the footprint and depth over the admissible tilt range (Cor. 7.8, whose range is supplied by Hypothesis 7.11 and not by the geometry); the orientation relation at all four combinations; and the closure ratio with its sensitivity. Appendix B.

Supposed. That the capped arm folds into one leaflet (Hypothesis 7.11), on which the leaflet map is defined at all; that units disperse rather than aggregate (Hypothesis 7.16); that the surface admits either presented face (Hypothesis 9.22); and the phosphatidyl reading of the head group (Supposition 6.7).

2 Status, nomenclature, scope

Convention 2.1 (Status labels)**.** [A] As in the coordinating paper. [A] finite or axiom-free; [D] derived under named hypotheses, registered in Appendix A; [C] imported, with the source named; [E] molecular reading, which enters no proof. Scholia carry no label and enter no proof.

Notation 2.2 (Locants)**.** [C] The locant ruling of the coordinating paper governs and is restated. The vessel graph X carries eighteen framework carbons on the cycle

$$1 - 2 - 3 - 4 - 4\mathrm{a} - 4\mathrm{b} - 5 - 6 - 6\mathrm{a} - 7$$
$$-8 - 9 - 10 - 10\mathrm{a} - 10\mathrm{b} - 11 - 12 - 12\mathrm{a} - 1,$$

together with three chords, C4*a*–C12*a*, C4*b*–C10*b* and C6*a*–C10*a*, which are the ring-fusion bonds and the interior connectors at which the corpus records scission. The substituted positions are C6 and C12. Statements written in the other convention are restated, not reconciled by context.

Notation 2.3 (The two tethers and their caps)**.** C Two tethers occur in the transformative synthesis and are imported unamended. Each unit carries its nucleoside on one arm and a capped arm at the other substituted position. The adenine unit:

$$\mathrm{C2(adenosine)-O\,CH_2CH_2\,O}$$
$$\mathrm{-P(=O)(O)-O\,CH_2CH_2\,O-C6,}$$

$$\mathrm{C12-O\,CH_2CH_2\,O-P(=O)(O)}$$
$$\mathrm{-O\,CH_2CH_2\,O-CH_2CH_3.}$$

The cytosine unit, whose nucleoside arm carries in addition a carboxyl- and nitrogen-bearing extension:

$$\mathrm{C5(cytosine)-C(COO)\,N\,C(OH)}$$
$$\mathrm{-O\,CH_2CH_2\,O-P(=O)(O)}$$
$$\mathrm{-O\,CH_2CH_2\,O-C6,}$$

$$\mathrm{C12-O\,CH_2CH_2\,O-P(=O)(O)}$$
$$\mathrm{-O\,CH_2CH_2\,O-CH(CH_3)CH_3.}$$

Write ℓ_{A} and ℓ_{C} for the number of bonds from base carbon to C6 along the nucleoside arm, and call the terminal alkyl group of the second arm the *cap*.

Lemma 2.4 (The arm inventory)**.** A $\ell_{\mathsf{A}} = 10$ *and* $\ell_{\mathsf{C}} = 13$*, the nucleoside arms differing by three backbone atoms. The caps are ethyl at the adenine unit and isopropyl at the cytosine unit: two carbons against three, linear against branched, and equal in backbone reach, the ethyl extending one atom further along the arm and the isopropyl standing wider at the same depth.*

Proof. Finite, by counting the backbones of Notation 2.3; Appendix B, block V5, computed. □

Remark 2.5 (Where the second datum resides)**.** A The arm inventory is the chemical half of what distinguishes one anchor from another, and it is not the whole. The remaining datum is not in the arms at all but in the body they hang from: the orientation of the aromatic system of the retained 6,12-disubstituted unit, taken against a reference that the cluster supplies and the unit does not carry in itself.
Three readings of that reference are available and they are not independent. Against the sequence's own external frame, the orientation is the datum β of Definition 4.7. Against the duplex the unit is tethered to, it is which of the two strands the unit's base belongs to, which is the same bit read locally. And the unit's position number along the segment orders the anchors, which is not a bit but is what makes a word of them rather than a bag.
The three are taken up in that order at Definition 4.7, Lemma 9.15 and Lemma 9.16. The distinction matters here only so that a reader does not look for the second datum among the caps, where it is not.

Remark 2.6 (Three data, in two senses)**.** A The anchors are separated by three data and the paper uses all of them. They differ in the length of the nucleoside arm, by three atoms. They differ in the carbon count of the cap, by one. They differ in the shape of the cap, linear against branched, which is not a difference of degree.
The second and third run opposite to the first. The cytosine unit carries the longer arm and the shorter, wider cap; the adenine unit the shorter arm and the longer, narrower cap. The differentiation is therefore two-dimensional, and the two letters are not related by a uniform lengthening of one object into the other. Remark 9.4 says what follows for the anchor word.

Convention 2.7 (Scope)**.** A The reference context is the 6,12-disubstituted unit, unrecruited where a lipid is at issue and tethered where an anchor is. One bridge topology is treated at a time, and no statement is transported between them except through Theorem 5.10, which is the statement that distinguishes them. No statement is made of the other substitution contexts of the corpus.

Convention 2.8 (Membrane, leaflet, face)**.** A The dominant substrate yields a bilayer and the minority substrate a monolayer former (Corollaries 5.16, 5.12). Sections 7 to 10 are written for the bilayer, which is what the dominant channel supplies and what the minority product is taken to span (Remark 5.14).
Should a reader wish to carry those sections to a membrane of the minority product alone, one substitution suffices: for *leaflet* read *face*, the two faces of a monolayer standing where the two leaflets of a bilayer do. Two statements then read differently. The leaflet map of Definition 8.1 becomes the record of which face a unit's nucleoside arm departs toward, and is defined without Hypothesis 7.11, a spanning species being the norm in a monolayer rather than an anomaly; and the lipid per vessel of Proposition 10.2 differs between the routes. Nothing else changes, the core-crossing count of Theorem 8.3 being the same across one slab as across a mid-plane.
The word *membrane* is used where either will serve, *bilayer* and *monolayer* only where the distinction bears.

Convention 2.9 (The regime)**.** [A] Every statement about a tethered unit in a surface is written in the dispersed regime of Hypothesis 7.16. Under aggregation the conclusions do not weaken; they change their subject, from units in a leaflet to units at a domain boundary, and Remark 7.17 says what that costs. Sections 5 and 6 are independent of the regime, concerning cut sets and counts.

3 Non-implications

Proposition 3.1 (Non-implications of this paper)**.** [A] *None of the following is asserted anywhere below.*

(i) That a cell is produced. A closed surface containing a strand is not a cell. Nothing here bears on metabolism, on division, on transport across the surface, or on replication, and no statement below should be read as supplying any of them.

(ii) That no material enters from outside. The head-group nitrogen and carbons of Supposition 6.7, and the thirty-two reducing equivalents of Proposition 5.19, are inputs. What is claimed is a ledger of what is and is not supplied, not a closed system.

(iii) That composition agreement is evidence. The agreement of total carbon between route A and a reference phosphatidylcholine is entailed by any account producing a forty-carbon phosphodiester amphiphile and discriminates nothing; and the oxygen, nitrogen and hydrogen counts are not constraints at all, by Convention 6.1. Scholium 3.2 says so at length, because this is the clause a reader is most likely to over-read.

(iv) That any spatial pattern of anchors persists. Lateral diffusion in a fluid bilayer destroys any arrangement of anchor positions. What survives is a pattern of orientations carried in strand order (Theorem 9.23), which is a different kind of object, and a composition (Corollary 9.38).

(v) That the chrysene unit is a sterol. The comparison is a reading, is labelled [E]*, appears in Appendix C and enters no numbered statement. The agreement in footprint recorded at Remark 7.9 is a coincidence of size between objects differing in planarity, saturation, chirality and anchoring.*

(vi) That the transformation occurs. Reachability is the non-emptiness of a hom-set. The four-level convention of the coordinating paper — connectivity, chemical admissibility, geometric accessibility and physical realization kept apart — is adopted here as this paper's, and no statement below asserts more than the level at which it is made.

Scholium 3.2 (Why (iii) is stated so early)**.** A paper that exhibits a forty-carbon dimer against a forty-carbon lipid is under pressure to present the agreement as a result about the architecture. It is not one, and the reason is better given as a positive statement than as a caution.

An elemental agreement is evidence only where the elements are scarce. Here three of the five are not: oxygen, nitrogen and hydrogen are admitted by generators the corpus already carries, and an account free to place them will place them wherever a comparand requires. An agreement reached under that freedom was not at risk, and a quantity not at risk carries no information. Only carbon is scarce, and carbon is scarce in a strong sense — eighteen per unit, four per bridge, and no generator that adds one.

So the ledger of Section 6 is a ledger in carbon, and even there the total is not the informative quantity. Two amphiphiles of equal total carbon and unequal partition differ in phase behaviour, which is the property the enclosure needs; the partition is what the architecture fixes, and the partition is what Theorem 6.4 reports. A reader who takes the coincidence of totals for the result has taken the part that was free for the part that was forced.

What the section is for, then, is an audit pointed inward. The dimer record is a declaration in the corpus; running the partition over it checks that declaration, and the value of the check is entirely in what a disagreement would have caught — a defect in the record, not in the architecture.

4 The reference architecture

This section states what is imported and fixes the objects the rest of the paper works on. Nothing here is established; every statement carries [C] or is a definition, and a reader who finds a claim in this section has found a drafting error.

Proposition 4.1 (The complex)**.** [C] *The encoding operates on a complex of two units: a 6,12-disubstituted chrysene paired with a 3,6,9,12-tetrasubstituted chrysene. The tetrasubstituted unit is the one that undergoes the transformation to a nucleobase of the nucleic acid. The disubstituted unit is the template on which that transformation is shaped, and it is not consumed: it remains tethered to the product it templated.*

Proposition 4.2 (The complex is doubly bridged)**.** [C] *The two units of a complex are joined at adjacent substituted positions of each, by phosphodiester bridges of the motif of*

Notation 2.3, so that catalyst and substrate together close a macrocycle. Imported from the synthesis pathway of the patent record [Sch25a], Figures 6, 7 and 9b, with the tethered complex at Figures 15a–c.

Proposition 4.3 (The fate of the two bridges)**.** [C] *On transformation of the substrate to a nucleobase, one bridge is retained and becomes the tether of Notation 2.3, joining the base to* C6 *of its template. The other is severed on the substrate side and terminated at the template, and what terminates it is the cap borne at* C12*.*

Corollary 4.4 (The cap is a record of the templating)**.** [C] *The cap is therefore not an arbitrary end group. It is the terminated remnant of the second catalytic bridge, and its identity — ethyl at one anchor type, isopropyl at the other — is written at the moment of templating by the same event that fixes α. Lemma 9.13 rests on this: the pair type is carried chemically because the chemistry that carries it is the chemistry that recorded it.*

Remark 4.5 (Why the macrocycle matters twice)**.** [A] The doubly bridged motif appears at two places in this paper and a reader should not run them together.
Here it is the geometry of the complex: catalyst and substrate closed into a macrocycle at adjacent positions, which is how the templating is held in register and which is consumed when the substrate becomes a base. That macrocycle is not available as material for a surface; it has already done its work.
At Section 5 the same bridging motif appears as a possible form of the *unrecruited* dimer, where it yields routes C and D of Theorem 5.10. The motif is the same and the object is not, and no statement about one is transported to the other.

Proposition 4.6 (The tethered unit)**.** [C] *The transformation of the encoded cluster yields an intercalated nucleic acid in which each anchored base retains, through the tether of Notation 2.3, the 6,12-disubstituted unit that templated it. The tether is therefore not an incidental attachment but a retained template contact, and the unit at its far end is the unit that shaped the base at its near end.*

Definition 4.7 (The orientational datum of a tethered unit)**.** [C] Each 6,12-disubstituted unit of a complex carries two binary orientational data, fixed at the moment it templated its partner:

- α, the alignment of its aromatic system to that of its paired tetrasubstituted unit — aligned or unaligned;
- β, the orientation of its rings in the reference frame common to the cluster.

The pair $(\alpha, \beta) \in (\mathbb{Z}/2)^2$ indexes base four *bijectively*: the map from orientation pairs to bases is one-to-one and onto, so that distinct orientations template distinct bases and every base is templated by one orientation. The indexing is the encoding.
The bijectivity is imported and is not derived here, and everything in Section 9 rests on it. Were the map not injective — were two orientations to template one base — the source entropy would fall below two bits per anchor and Theorem 9.23 would be measured against the wrong source. Remark 9.26 states the disposition: a reader who denies the identification denies the source, not the injection.

Remark 4.8 (The anchor is not a label on the sequence but a carrier of it)**.** [A] The consequence for this paper should be stated explicitly at the outset, since an earlier draft reversed it and the correction propagates through every later section. A tethered unit is not a tag attached to a nucleic acid after the fact. It is the object whose orientation determined which base was made, and it holds that orientation still. Two units at two positions of a strand differ in (α, β) exactly as the bases they templated differ, and they differ in it as a matter of their own geometry rather than by reference to the strand. So when a tethered unit migrates into a surface it does not carry a pointer to an encoding held elsewhere. It carries the encoding. What Section 9.2 asks is therefore not whether a label survives the passage but how much of a two-bit-per-anchor source a surface can hold, and Theorem 9.23 answers it.

Proposition 4.9 (The unrecruited dimer)**.** [C] *Units of the 6,12-disubstituted family not recruited into a complex occur as dimers, bridged at a substituted position by a phosphodiester of the same motif as the tethers:*

$$\mathrm{C12(X}_n\mathrm{)-O\,CH_2CH_2\,O-P(=O)(O)}$$
$$\mathrm{-O\,CH_2CH_2\,O-C12(X}_{n+1}\mathrm{)},$$

the patent record exhibits this dimer at [Sch25a], Figure 16b. Where both substituted positions are bridged the dimer closes as a macrocycle, by the motif of Proposition 4.2.
The dominant motif is the singly bridged form: one substituted position of each unit carries the bridge and the other carries its ether oxygen, free. A minority of dimers are bridged at both positions and close a macrocycle, by the motif of Proposition 4.2 and as exhibited at [Sch25a],

Figure 16b. The two forms are treated together in Section 5 and are distinguished there by Theorem 5.10; the proportion between them is not supplied by the record and is not estimated here.

Remark 4.10 (What each substrate settles)**.** [A] The form of the substrate decides which routes of Theorem 5.10 have anything to run on, and the two forms decide differently.
The singly bridged form leaves C6 free, so an ether stands at that position and may be eliminated. Route A runs on it, its product is a di-*O*-(octadec-9-enyl) phosphate, and the membrane is a bilayer.
The macrocycle leaves no ether free, so no elimination is available on it (Remark 5.15); routes C and D run on it, and route C yields a bolaamphiphile, which forms a monolayer rather than a bilayer (Corollary 5.12).
Since the first form is dominant, the membrane of this paper is a bilayer and the monolayer former is a minority component within it. Remark 5.14 says what such a component does there.

Proposition 4.11 (The substrates of Sections 5 and 6)**.** [C] *Two substrates are carried. The dominant one is the singly bridged dimer*

$$\mathrm{C12(X}_n\mathrm{)-O\,CH_2CH_2\,O-P(=O)(O)}$$
$$\mathrm{-O\,CH_2CH_2\,O-C12(X}_{n+1}\mathrm{)},$$

with C6 *of each unit carrying its ether oxygen and no further bridge. The minority one is the macrocycle bridged at both positions, in which no ether is free.*

Remark 4.12 (Why the minority form is carried)**.** [A] A paper concerned only with the dominant motif would state one form. Both are carried because they yield different membranes — a bilayer and a monolayer former — and because the minority product has a use in the majority membrane that neither has alone (Remark 5.14). The proportion is a target and not a result.

Convention 4.13 (Unrecruited, not unencoded)**.** [A] The dimer of Proposition 4.9 is called *unrecruited* throughout: it was not drawn into a complex and templated no base. The corpus and the patent record call it unencoded, and an earlier draft of this paper followed them; the word is retired here because it misdescribes the object. The dimer is not of a family unrelated to the encoding. It is of the same family as every tethered unit, and differs from one only in never having been drawn into a complex.

The distinction matters twice below. At Section 6 it is why the lipid and the anchor have the same carbon skeleton, which is not a coincidence but an identity of family. At Section 7 it is why a tethered unit partitions into a surface of these lipids at all: the surface is made of its own kind, unscissioned.

Definition 4.14 (The pool)**.** [D] Let $\mathcal{P}$ be the units of the 6,12-disubstituted family available to an assembly, partitioned into those recruited into complexes and those not. Write ν for the number of unrecruited vessels per encoded vessel. It is the parameter Theorem 10.5 computes, and Corollary 10.6 is a condition on the setting rather than a property of the architecture.

Remark 4.15 (Why both bridge topologies are carried)**.** [A] A paper needing only one of them would state one. Both are carried because Theorem 5.10 finds that the bridge count does not by itself decide the product: the macrocycle reaches the same diacyl topology as the single bridge, at a different cut count and with different tails, and is excluded by tail length rather than by topology. That finding is unavailable to an account that fixes the bridge topology in its architecture section.

Convention 4.16 (What is not imported)**.** [A] The seeding and refinement apparatus, the assignment machinery, the registry capacity and the parity obstruction are not drawn on. This paper takes the tethered units of Proposition 4.6 with the datum of Definition 4.7, and a pool of unrecruited dimers, and asks what surface they make and what of the datum the surface holds. No statement below turns on which assignment the registry supports.

5 Scission of the unrecruited dimer

The object of this section is the object the corpus already cuts: the vessel graph with its eighteen-cycle and three chords, under a subset of its edges. What differs is the target. The excision of the residue account carves a retained subgraph rooted at C5; the scission here carves a path. Whether the two are the same generator under different cut sets is a coordination question and is put at Remark 13.5.

The section is finite throughout. Every cut set is enumerated, and the statements below are transcribed from blocks V1, V2 and V2b rather than asserted.

Definition 5.1 (Cut set)**.** [D] A cut set $\mathcal{K}$ is a subset of the edge set of X, and $\mathsf{X} \setminus \mathcal{K}$ is the graph it leaves. By

Notation 2.2 X carries eighteen vertices, eighteen cycle edges and three chords, and the substituted vertices are C6 and C12. A cut set is *chain-forming* if every component of $X \setminus \mathcal{K}$ is a path.

Definition 5.2 (Attachment). [D] A component of $X \setminus \mathcal{K}$ is *attached* if it contains a substituted vertex, and *terminally attached* if it contains one as an endpoint. A component containing no substituted vertex bears no polar group and is an unattached alkane; it is counted and is not part of any amphiphile.

Lemma 5.3 (The cut count is forced). [A] X *carries eighteen vertices and twenty-one edges, so its cyclomatic number is* $21 - 18 + 1 = 4$*, which is the ring count of the skeleton. A chain-forming cut set therefore severs at least four edges, and four suffice.*

Proof. Finite; Appendix B, block V1b, computed. □

Remark 5.4 (Three of the four are the corpus's own). [C] The three chords C10*a*–C6*a*, C10*b*–C4*b* and C12*a*–C4*a* are the interior connectors at which the corpus already records scission activity. Severing them is therefore not a choice made here but a transport of the corpus's own loci, and by Lemma 5.3 it leaves the eighteen-cycle and exactly one further edge to be chosen.
The consequence narrows the section considerably and is stated here explicitly. The cut set is forced up to one edge among eighteen; every statement of Section 5 is an enumeration over that one choice, and Theorem 5.6 finds four of the eighteen admissible.

Lemma 5.5 (A chain of eighteen). [A] *Severing the three chords together with one cycle edge leaves a Hamiltonian path on the eighteen framework carbons. There are eighteen such cut sets and each leaves a single unbranched chain of eighteen carbons, the endpoints being the two ends of the severed edge.*

Proof. Finite, over the edge inventory; Appendix B, block V1, computed. □

Theorem 5.6 (Terminal attachment). [A] *A chain-forming cut set of Lemma 5.5 is terminally attached at a substituted vertex if and only if the severed cycle edge is incident to that vertex. There are exactly two such cut sets at* C6*, namely* {C5–C6} *and* {C6–C6*a*}*, and exactly two at* C12*, namely* {C11–C12} *and* {C12–C12*a*}*. No cut set of this kind is terminally attached at both.*

Proof. Finite; Appendix B, block V1, computed. The last clause is immediate: the endpoints of the path are the ends of the severed edge, and C6 and C12 are not adjacent in the cycle. □

Proposition 5.7 (The position of the remaining substituted vertex). [A] *In each of the four cut sets of Theorem 5.6 the other substituted vertex lies at position nine of the eighteen, measured from the terminal one. Hence the chain is divided by it into segments of nine and eight carbons.*

Proof. Finite; Appendix B, block V2b, computed. □

Proposition 5.8 (Two chains from one vessel). [A] *Severing the three chords together with two cycle edges yields one hundred fifty-three cut sets, each leaving two chains of lengths* k *and* $18 - k$*. Of these, eighty-one separate* C6 *from* C12*, and exactly two separate them with each terminal in its own chain:*

{C5–C6, C11–C12} *and* {C6–C6*a*, C12–C12*a*}*,*

each leaving two chains of nine. Exactly two further cut sets leave both substituted vertices terminal in one chain of ten, together with an unattached chain of eight.

Proof. Finite; Appendix B, block V2, computed. □

Definition 5.9 (Amphiphile topology). [D] Let a bridge be a phosphodiester joining substituted vertices of two units. The *topology* of the product is the isomorphism type of the tree formed by contracting each bridge to a vertex and each chain segment to an edge, recorded together with the multiset of tail lengths, a tail being a maximal segment of a chain not meeting a bridge.

Theorem 5.10 (The admissible routes). [A] *Under Definition 5.2 and the two bridge topologies of Proposition 4.9, the chain-forming cut sets leaving no unattached chain realise exactly four topologies:*

route	*br.*	*cuts*	*topology*	*tails*
A	*1*	*1*	*diacyl*	18, 18
B	*1*	*1*	*tetra-alkyl*	9, 8, 9, 8
C	*2*	*1*	*cyclic bola*	*ring* + 8, 8
D	*2*	*2*	*two diacyls*	9, 9 *each*

"br." is the number of bridges and "cuts" the cycle cuts per unit; route C's

tails are pendant on the ring. *Routes A and B differ only in which of the two substituted vertices the severed edge is incident to, by Theorem 5.6; routes C and D differ in the number of cuts per unit, by Proposition 5.8.*

Proof. Finite, over the enumeration of Lemma 5.5 and Proposition 5.8, with the position of Proposition 5.7; Appendix B, blocks V2 and V2b, computed. □

Remark 5.11 (Which routes have substrate)**.** [A] The enumeration of Theorem 5.10 is over cut sets and is finite whatever the record exhibits. The four routes divide by substrate.

Routes A and B run on the singly bridged dimer, which is the dominant form (Proposition 4.11). Routes C and D run on the macrocycle, which is the minority form, exhibited at [Sch25a] Figure 16b. Both substrates are present; the proportion between them is not supplied by the record.

The account is accordingly written for the dominant channel, and the minority channel is carried alongside it at Corollary 5.12 and Remark 5.14.

Corollary 5.12 (What the minority substrate yields)**.** [A] *On route C the product is a macrocycle of twenty-eight ring carbons — ten framework carbons from each unit together with the eight of the two bridges — carrying two phosphorus centres diametrically placed and two pendant tails of eight carbons. Fourteen carbons separate the two phosphorus centres along either arc.*

This is a macrocyclic bolaamphiphile: two polar centres on one ring with hydrophobic arcs between them. Such an amphiphile spans a membrane once and forms a monolayer*, not a bilayer.*

Proof. Finite; Appendix B, block V2b, computed. □

Corollary 5.13 (The thickness of the monolayer)**.** [A] *The hydrophobic thickness of a route-C membrane is at most the extended span of one arc,* $14 \times 1.27 = 17.8$ *Å, and less as the arc bows: about* 15 *Å lightly bowed. This is thinner than an archaeal tetraether monolayer at* 25 *to* 30 *Å and than a di-*C18:1 *bilayer at* 27*.*

Proof. Finite; Appendix B, block V2b, computed at three degrees of bowing. □

Remark 5.14 (The minority product spans the majority membrane)**.** [A] A bolaamphiphile placed in a bilayer does not form a phase of its own at low mole fraction. It spans the bilayer, presenting a head at each interface, and in doing so couples the two leaflets mechanically — which is the structural role archaeal bolalipids play where they occur alongside bilayer-forming species.

The office requires a fit the macrocycle does not have at rest. By Corollary 5.13 it spans about fifteen Å against the twenty-seven of a di-C18:1 bilayer: a shortfall of twelve Å, which is not a thinning but nearly half the thickness. A bilayer does not accommodate that by local compression.

Two readings remain and the paper adopts neither. Either the macrocycle segregates, at any mole fraction, into a domain of its own of the monolayer thickness of Corollary 5.13, with a boundary against the bilayer — in which case it is not a staple but a second phase. Or it spans a bilayer thinned by some other means to about fifteen Å, which no component of this architecture supplies. The stapling reading is therefore recorded as unavailable on the present geometry, and what survives is the weaker statement that the minority substrate yields an amphiphile of a membrane-forming class rather than waste. Target 14.4 asks for the mole fraction and the phase behaviour.

What can be said is that the minority product is not waste. It is a species of the right topology to staple the leaflets of the membrane the majority product forms, and an architecture that made both from one pool would be making a membrane and a cross-link for it from the same material.

Remark 5.15 (No free ether on the minority substrate)**.** [A] In the macrocycle both substituted positions carry a bridge, so no ether is free. The elimination of Theorem 5.20, which places a double bond at Δ9 because the C6 ether stands at carbon ten of eighteen, has no substrate on routes C and D; their arcs and tails are saturated, or carry unsaturation the reduction ledger does not locate.

The Δ9 result belongs to the dominant substrate and is stated there without condition. The minority channel is unsaturated at no fixed position, and nothing below asks it to be.

Corollary 5.16 (The bilayer selects route A)**.** [A] *Of the four routes only A places its tails in the range within which a diacyl amphiphile forms a lamellar phase. Route D reaches the diacyl topology at tails of nine, which is the micelle-forming range; route B distributes the same carbon over four tails of eight and nine, a high-curvature geometry; route C is a macrocycle and forms a monolayer.*

Route A runs on the dominant substrate, so the membrane of this paper is a bilayer of its product, and the minority channel contributes the spanning species of Remark 5.14 rather than a second phase.

Remark 5.17 (The selection is by length, not by topology)**.** [A] Within the diacyl class the selection is by tail length and not by topology: route D reaches that topology from the same macrocyclic substrate as route C, at two cuts per unit rather than one, and is excluded by its tails of nine and not by its shape. The bridge count does not decide the product and neither does the topology alone. What decides it is a cut set, and the four admissible cut sets are named at Theorem 5.6 and Proposition 5.8.

5.1 The fate of the ether, and the unsaturation it leaves

Remark 5.18 (The ether stands mid-chain)**.** [A] A consequence of Proposition 5.7. On route A the tail is terminally attached at C12, which is carbon one, and C6 stands at carbon ten of eighteen — as near the middle as an even chain permits. The architecture therefore does not place this oxygen at will. Its position is fixed by the cut set, and it is fixed near the mid-plane of the leaflet.
Two fates are then available to it: retention, leaving a mid-chain ether, or elimination, leaving a double bond. The second is treated below and is the one the paper adopts.

Proposition 5.19 (The reduction ledger)**.** [A] *The skeleton is* $C_{18}H_{12}$ *and carries thirteen degrees of unsaturation: four rings and nine carbon–carbon double bonds. The four rings are discharged by the cut set, by Lemma 5.3. Of the nine double bonds, eight are reduced and one is retained, by Theorem 5.20; the reduction charged is sixteen hydrogens per tail and thirty-two per dimer.*

Proof. Finite; Appendix B, block V3b, computed. □

Theorem 5.20 (The position of the retained unsaturation)**.** [A] *On route A, let the ether borne at* C6 *be eliminated in the course of the scission rather than reduced. Numbering the chain from* C12 *as carbon one,* C6 *is carbon ten in both admissible cut sets, and elimination toward* C5 *leaves a double bond between carbons nine and ten. The retained unsaturation is therefore at* Δ9 *and the tail is octadec-9-en-1-yl. Elimination toward* C6*a leaves it at* Δ10*. No other position is reachable, the ether standing at a single carbon with two chain neighbours.*

Proof. Finite; Appendix B, block V2c, computed at both admissible cut sets and both elimination senses. □

Corollary 5.21 (The route-A product, named)**.** [A] *Under Theorem 5.20 at* Δ9 *the route-A product is*

$$\mathrm{R-O\,CH_2CH_2\,O-P(=O)(OH)-O\,CH_2CH_2\,O-R},$$
$$\mathrm{R} = \textit{octadec-9-en-1-yl},$$

of formula $C_{40}H_{79}O_6P$*: a dialkyl phosphate diester with two ether-linked mono-unsaturated tails of eighteen carbons.*

Proof. Finite; Appendix B, block V3b, computed. □

Remark 5.22 (The locus is shared with the residue account)**.** [A] The edge across which the elimination runs to give Δ9 is C5–C6, which is the edge the residue account severs at sixteen of its nineteen rows. One edge is therefore the reactive locus of both branches of the arc: severed, it releases the side chain of a residue; eliminated across, it fixes the unsaturation of a tail.
What this is worth should be said carefully, because it is easy to take for more than it is. It is a coincidence of locus and not a mechanism. Nothing here shows that the two operations are the same operation, and nothing shows that an architecture performing one must perform the other. What it shows is that the two branches make their respective products at the same bond, which is a fact about the skeleton. It is the content of Remark 13.5 stated concretely, and the coordination question it raises is Target 14.12.

Remark 5.23 (What the architecture does not fix)**.** [A] Two things about the retained unsaturation are left open and they are not of equal weight.
The first is the choice between Δ9 and Δ10, which is the sense of the elimination. Either is a mono-unsaturated eighteen-carbon tail and either is lamellar; the distinction bears on the comparand and not on the enclosure.
The second does bear. A *cis* double bond at Δ9 introduces the kink that keeps an eighteen-carbon tail fluid at ordinary temperatures; the *trans* isomer packs very nearly as the saturated chain does and raises the transition temperature by tens of degrees. Nothing in the enumeration selects between them. A *trans* product would refute no statement of this paper and would make two of its premises false at once — Hypothesis 7.16 and the lateral diffusion on which Proposition 3.1(iv) rests — leaving an account of a gel-phase object rather than of a membrane. It is entered as Target 5.25.

Target 5.24. (Aggregated at Target 14.6.) Decide between retention and elimination at the C6 ether. Under retention the tail carries a mid-chain ether at carbon ten; under elimination

it carries a double bond there. The question belongs to the certification layer and bears on Corollary 5.21.

Target 5.25. (Aggregated at Target 14.6.) Determine the geometry of the double bond of Theorem 5.20. The question decides whether route A yields a fluid lamellar phase or a gel, and with it whether Hypothesis 7.16 is available at all.

6 The composition ledger

Convention 6.1 (What the ledger counts)**.** [A] Oxygen, nitrogen and hydrogen are admitted elsewhere in the architecture — in the scission itself, in the phosphodiester, and in the nucleic-acid synthesis — and are available to be placed where a structure requires them. They are therefore not constraints and are not counted here. Carbon is not so available: the framework carbons of a unit are fixed at eighteen and the linker carbons at four, and no generator of the corpus adds a carbon. The ledger of this section is accordingly a ledger in carbon alone, and its question is the partition and not the total.

Proposition 6.2 (The carbon budget)**.** [A] *The carbon available to one dimer is thirty-six framework carbons together with four linker carbons per bridge: forty under the single bridge and forty-four under the macrocycle. Route A partitions its forty as four in the linker and thirty-six in two tails of eighteen; route D partitions its forty-four as two lipids of twenty-two, each four in the linker and eighteen in two tails of nine.*

Proof. Finite; Appendix B, block V3, computed. □

Proposition 6.3 (The route-C partition)**.** [A] *The macrocycle of Corollary 5.12 carries forty-four carbons: twenty-eight in the ring, of which eight are linker, and sixteen in the two pendant tails. Its two phosphorus centres lie at the ring's two polar positions.*
Against a macrocyclic archaeal lipid the partition is of the same kind — a ring bearing two heads with hydrophobic arcs between — and differs in scale, fourteen carbons to an arc against the twenty to twenty-five of that class.

Proof. Finite; Appendix B, blocks V2b and V3, computed. □

Theorem 6.4 (The partition against reference amphiphiles)**.** [A] *The route-A product of Corollary 5.21,* $C_{40}H_{79}O_6P$*, is a di-O-(octadec-9-enyl) phosphate. It does not approximate that class; it is a member of it, in partition, in tail length, in unsaturation and in linkage, and that class is lamellar.*
It is not a phosphatidylcholine. A phosphatidylcholine of the same total carbon partitions it as eight and thirty-two, spending three carbons on a glycerol and five on a choline and carrying one nitrogen; matching it requires four carbons moved from tail to head, which no generator supplies. Against a dioleoyl phosphatidic acid the difference is the linkage — ether where that class has ester — and two oxygens.

Proof. Finite; Appendix B, block V4, computed, against the comparands printed there. □

Remark 6.5 (What the naming buys)**.** [A] A ledger that returns a class rather than an approximation carries more information than its arithmetic alone, because the class was not selected in advance. The tail length is forced by the framework at eighteen; the unsaturation is forced by the ether at carbon ten; the linker is forced by the bridge at four carbons; the linkage is an ether because the arm was an ether. Each was fixed before any comparand was consulted, and the four together land inside a class that exists and forms bilayers.
That is a different kind of statement from the total-carbon agreement of Remark 6.8, and a reader should keep the two apart. The second was free; this one was not.

Corollary 6.6 (The membrane does not rest on the head group)**.** [D] *Route A is bilayer-forming and route C monolayer-forming, both as they stand and neither resting on a head-group identification. Every statement of Sections 7 to 10 requires a lamellar surface and no statement of them requires a phosphatidyl head group, so the enclosure of this paper is independent of the identification at Supposition 6.7.*

Supposition 6.7 (The phosphatidyl reading)**.** [D] Suppose a glycerol and a choline are supplied to the linker, the nitrogen by the generator that supplies the α-nitrogen of the residue account and the carbons from outside the dimer. Then the product is a phosphatidylcholine.
This is a supposition and is stated where it is used. It is registered as H1 in Appendix A. It is not derived here and is not derived anywhere in the corpus.

Remark 6.8 (What the coincidence is and is not)**.** [A] That route A and a reference phosphatidylcholine carry the same total carbon is a fact and is worth recording, and it is not

evidence. Two amphiphiles of the same total carbon and different partitions are different molecules with different phase behaviour, and the partition is the part that bears on the bilayer. The agreement of the totals is entered at block V4 and is given no further weight.

The statement that does bear is Corollary 5.16: the tails of route A fall in the lamellar range. That is a statement about the enumeration of Section 5 and not about any comparand.

Remark 6.9 (Where the supposition sits)**.** [A] An earlier framing of this arc had the enclosure arise without exogenous material. That framing is unavailable and is withdrawn at Remark D.2. The honest statement is narrower and holds: the enclosure arises without material beyond what the architecture already admits, and the head-group identification arises only with carbon that it does not. The first is the paper's; the second is Supposition 6.7's, and Corollary 6.6 is the reason nothing below depends on it.

7 Siting of the tethered unit

The preceding sections carve a lipid and say nothing about the unit that was tethered. This section places it in the surface. It is the paper's most physical section and its least secure, and the two facts are related: what can be computed here is geometry, and what cannot be computed is whether the geometry is tolerated.

Everything Sections 8 and 9 assume about the tethered unit — that it occupies one leaflet, that the leaflet is a well-defined datum, that the unit is oriented across it — is established here or nowhere.

Proposition 7.1 (Amphiphile by topology)**.** [D] *The phosphodiester of each arm is polar and the polycyclic skeleton is apolar, and the two are adjacent along the arm. Partition therefore places the phosphodiester at the interface and the skeleton in the acyl core. The argument is from the topology of the molecule and uses no resemblance to any other.*

Remark 7.2 (The surface is made of the unit's own kind)**.** [A] There is a second and simpler reason to expect the tethered unit in the surface, and it is available only because of Convention 4.13.

The lipid of Corollary 5.21 is an unrecruited 6,12-disubstituted unit that has been cut and reduced. The tethered unit is a 6,12-disubstituted unit that has not been. They are the same skeleton bearing the same phosphodiester arms, differing in whether the four rings have been opened. The tethered unit is therefore not a foreign body inserted into a membrane of some other substance — the case a sterol comparison would have it in — but the uncut form of the membrane's own material, sitting among the cut form. This disposes of a question the section would otherwise have to argue: whether a polycyclic aromatic is tolerated in an acyl core at all. The core is made of chains that were that aromatic. What remains at issue is not the chemistry of the insertion but its geometry, which Propositions 7.3 and 7.6 address, and its aggregation, which Hypothesis 7.16 does not settle.

Proposition 7.3 (The skeleton, measured)**.** [A] *On an ideal hexagonal lattice with aromatic* C–C *at* 1.40 *Å, the four cata-condensed rings of the chrysene zigzag place eighteen carbons with extents* 9.10 *Å along the long axis and* 3.64 *Å across it; with a van der Waals envelope,* 12.50 *Å and* 7.04 *Å. The plane presents a thickness of* 3.40 *Å at π contact.*

Proof. Finite, by construction; Appendix B, block V8, computed. The construction recovers eighteen distinct carbons, which is the check that the embedding is the skeleton of Notation 2.2 and not another tetracycle. □

Lemma 7.4 (Where the substituted positions are)**.** [A] C6 *and* C12 *stand at cycle distance nine on the eighteen-cycle, which is half of it; but they are not at opposite ends of the long axis.* C6 *lies on ring C and* C12 *on ring B, the two interior rings. Their separation is* 5.05 *Å and the vector joining them lies at* 46° *to the long axis, with components* 3.50 *Å along it and* 3.64 *Å across it.*

Proof. Finite, by an embedding whose locants are recovered from the chord pattern C4*a*–C12*a*, C4*b*–C10*b*, C6*a*–C10*a* rather than assigned by hand; Appendix B, block V8, computed. □

Remark 7.5 (A correction, and what it cost)**.** [A] An earlier form of this section argued from cycle antipodality that the two arms leave from opposite ends of the long axis, and concluded that the long axis lies along the bilayer normal. The conclusion does not follow and the premise is false as a geometric statement: antipodality on the cycle is a property of the perimeter walk and not of the embedding, and the walk passes through the interior rings on its way. The correction is entered at Remark D.5.

It matters in the favourable direction. The skeleton presents less depth about the C6–C12 axis than about its long axis, and the arm budget of Remark 7.10 is correspondingly relieved.

Proposition 7.6 (The orientation is constrained and not determined)**.** [D] *Assume Propositions 7.1 and 9.6. The nucleoside arm leaves* C6 *or* C12 *for the interface and the capped arm leaves the other for the core, so the bilayer normal must have a non-vanishing component along the* C6–C12 *vector, which by Lemma 7.4 is neither the long axis nor the short one.*
Write ϕ for the angle of the normal within the molecular plane, measured from the long axis. That requirement excludes exactly one tilt: the normal may not stand perpendicular to the C6–C12 *vector, which on the embedding of Lemma 7.4 occurs at $\phi = 43.9°$, where the depth separation of the two substituted positions vanishes. The requirement therefore constrains the orientation without determining it, and it is weaker than a window: away from that one angle every tilt separates the two positions, and the separation rises to* 3.50 *Å at $\phi = 0°$ and to* 3.64 *Å at $\phi = 90°$.*
The free parameter is a tilt within the plane. It is not the presented face of Definition 9.19, which is a choice of which side of the plane faces outward; nothing in Section 9.2 depends on the tilt.

> *Proof.* Finite, by the embedding; Appendix B, block V8, computed. The excluded angle is the one at which the normal is perpendicular to a vector lying at 133.9° to the long axis. □

Remark 7.7 (A second correction to this section)**.** [A] An earlier form of Proposition 7.6 confined the normal to a window of some 44°, between the short-axis direction and the C6–C12 direction at 46°. Neither endpoint survives.
The 46° of Lemma 7.4 is the angle between two *lines* and is correct as such; the C6–C12 vector itself lies at 133.9° to the long axis. Taking the line angle for a direction put the window's lower endpoint within three degrees of the one tilt the criterion forbids: at $\phi = 46°$ the depth separation is 0.18 Å, which is the smallest value it takes anywhere, not the largest. The argument of the proposition yields no window at all, only an excluded angle.
What supplies a range is not that argument but the requirement that the unit occupy one leaflet, and that requirement rests on Hypothesis 7.11 rather than on the geometry alone. The range is therefore stated at Corollary 7.8 as a consequence of H7, and is labelled accordingly. The correction is entered at Remark D.6.
It moves no figure. The intervals of Corollary 7.8 and the budget of Remark 7.10 were computed over the range H7 supplies and are unchanged; it is the derivation, and not the arithmetic, that was at fault.

Corollary 7.8 (Footprint and depth, over the admissible tilt range)**.** [D] *Assume the unit lies within one leaflet, which H7 and Corollary 7.13 below supply. For it to do so, the skeleton's depth along the normal together with the capped arm folded to its freely jointed extent of* 3.8 *Å must not exceed the* 13.5 *Å hydrophobic half-thickness. The depth is therefore at most* 9.7 *Å, which by the sweep confines the tilt to $\phi \gtrsim 68°$: a range of some* 22°*, abutting the short-axis direction.*
Across that range the skeleton presents a depth of 7.0 *to* 9.7 *Å and a footprint of* 0.39 *to* 0.43 *nm^2. The depth is between fifty-two and seventy-two per cent of the hydrophobic thickness of one leaflet of a di-*C18:1 *bilayer; the footprint is between* 1.9 *and* 2.1 *acyl-chain cross-sections. The two move oppositely: the shallowest disposition is the widest.*

> *Proof.* Finite, by sweeping the tilt; Appendix B, block V8, computed at seven angles and at the threshold. The range is the one on which the depth criterion above holds; it is not supplied by Proposition 7.6, which excludes a single angle and no more. See Remark 7.7. □

Remark 7.9 (The footprint agrees with a sterol, and this is not used)**.** [A] The footprint of Corollary 7.8 brackets the 0.38 nm^2 usually given for a cholesterol ring system, and the agreement is closer than the earlier and incorrect figure of 0.24 nm^2 suggested. It is recorded because it is true and because a reader will find it, and it is used nowhere. Remark 7.18 says why a footprint agreement does not license the rest of the comparison; an agreement in one dimension between objects differing in planarity, saturation, chirality and anchoring is a coincidence of size.

Remark 7.10 (The arm budget, and what it threatens)**.** [A] The geometry above leaves a difficulty which is the most serious in this section and which is stated here rather than deferred.
Fully extended, the unit measures 30 to 33 Å from the base attachment to the cap: eleven for the nucleoside arm, seven to ten across the skeleton, eleven for the capped arm. The hydrophobic core of the bilayer is about 27 Å thick. A fully extended unit is therefore still longer than the core it is supposed to sit in, and were both arms extended it would deliver its cap to the far interface — that is, it would span the bilayer, and the leaflet map of Definition 8.1 would not be defined at that anchor.
The cap is apolar and will not stand at an aqueous interface, so the extended disposition is not the one adopted. The capped arm folds back into the core, and on the present geometry it need lose only 2.8 to 5.5 Å of its eleven to bring the unit within one leaflet — against the eight and a half the

earlier and incorrect geometry demanded. A freely jointed estimate of its end-to-end extension is $\sqrt{9} \times 1.27 = 3.8$ Å, which is to say that the arm gives up some 7.6 Å of its extension unforced; that is more than the 5.5 Å the shallowest admissible tilt asks of it, and the margin is the widest at the deepest tilt. The requirement is met across the range with room in hand.

The premise is therefore much more comfortable than it was two paragraphs of drafting ago, and it is still a premise. The paper rests on it rather than proving it.

One reading relieves it and is worth recording though the paper does not adopt it. In a membrane of the minority product (Convention 2.8) the hydrophobic region is a single slab of some fifteen Å rather than two leaflets of thirteen and a half, and a species spanning it is the normal case rather than an anomaly; the failure mode Hypothesis 7.11 guards against does not arise there in the same form. The dominant channel gives a bilayer, so the premise stands as stated.

Hypothesis 7.11 (The capped arm folds)**.** [D] The capped arm adopts a folded rather than an extended disposition, so that the unit together with both arms is contained within one leaflet. Registered as H7 in Appendix A.

Remark 7.12 (H7 and H8 may be antagonistic)**.** [A] Hypothesis 7.11 and Hypothesis 9.22 are settled by one enumeration — the rotamer states of a nine-atom phosphodiester arm — and an earlier form of this paper took that as a reason to expect them to stand or fall together. It is also a reason to expect them to compete, and the second reading is not excluded here.

H7 requires the capped arm to be *collapsed*: the freely jointed estimate of 3.8 Å against 11.4 Å extended is an estimate of a chain that has given up most of its reach. H8 requires the nucleoside arm to be *free* enough to deliver its base to the interface from either face of the skeleton. The two arms are distinct, so no contradiction is immediate. But they leave the same unit within one leaflet of finite depth, and conformational freedom spent on folding one is not available to the other in the space that remains.

If the folding H7 needs is what removes the freedom H8 needs, the account obtains its subject at the cost of its capacity: Sections 8 and 9 would have an object, and the channel would carry one bit per anchor rather than two. Nothing here shows that, and nothing here shows the reverse. What is recorded is that the conjunction H7 $\wedge$ H8 is a stronger premise than either conjunct, that the paper assumes the conjunction, and that Target 14.1 must return a rotamer population satisfying both rather than each in turn.

Corollary 7.13 (The unit occupies one leaflet)**.** [D] *Under Hypothesis 7.11 the unit does not span the mid-plane, and the leaflet map of Definition 8.1 is defined at every anchor. This is the premise Section 8 requires and Section 9.2 uses, and it is supplied here and nowhere else.*

Remark 7.14 (What fails with H7)**.** [A] More than any other premise of this paper, and it is worth recording where. If the capped arm does not fold, the unit spans the bilayer; λ is not a function on anchors; Theorem 8.3 has no subject; Theorem 9.23 loses the term it is an identity in; and the whole of Sections 8 to 9.2 is about an object that does not exist.

What survives is Sections 5 and 6 entire — the scission, the routes, the unsaturation, the ledger — which concern the unrecruited dimer and not the tethered unit, and Section 10's closure arithmetic, which needs a surface and a strand but not an anchoring of this kind. That is a substantial account and it is not the account this paper set out to give.

H7 is therefore the premise to settle first, ahead of H8 and ahead of the cap geometry. It is entered at Target 7.15.

Target 7.15. (Aggregated at Target 14.1.) Determine whether the capped arm folds into one leaflet or extends across the core. The question is conformational, is finite once the arm's rotamer states are enumerated, and decides whether the leaflet map is defined at all.

Hypothesis 7.16 (The dispersed regime)**.** [D] Tethered units are dispersed in the surface rather than aggregated into a domain. Registered as H2 in Appendix A.

Remark 7.17 (The cohesion tension)**.** [A] The π-stacking that holds the cluster together works against dispersal: rigid planar aromatics in an acyl core aggregate, and Corollary 7.8 gives the unit a footprint of about two chains and a face of 12.5×7.0 Å available for stacking, which is a large contact area to leave unused. The face stands with the normal in its plane, by Proposition 7.6, so the contact available to two neighbouring units is lateral and face to face — the disposition in which aromatics stack.

The paper assumes the dispersed regime and does not establish it. Under aggregation the anchors of a strand are not independently placed, the leaflet map is evaluated at a domain boundary rather than within a leaflet, and the statements of Section 9.2 are made of units whose faces are in contact with one another rather than with the core. That is a different object and not a weaker version of this one.

The prior runs against the hypothesis and should be stated

explicitly. The interaction assumed away here is the interaction the corpus's architecture is built on: π-stacking of these same units is what holds a cluster together and is what the encoding is registered against. An assembly that stacks them everywhere else is not obviously one that disperses them in an acyl core. H2 is therefore not one premise among eight but the one whose prior is unfavourable, and it is placed second in Section 14.1 for that reason.

Remark 7.18 (The sterol comparison, and why it is not used)**.** [E] A reader will reach for cholesterol, and the comparison is natural enough: a fused tetracyclic standing in a leaflet with a polar attachment at one end. Corollary 7.8 even puts the two within a factor of two in footprint and gives them a comparable span.
It is not used here and enters no numbered statement. Cholesterol is non-planar, largely saturated, chiral at eight centres, and anchored by a hydrogen-bonding hydroxyl that sits at a definite depth; the chrysene unit is planar, aromatic, achiral in its skeleton, and anchored by a phosphodiester at the end of a flexible arm. The behaviour a sterol is known for — ordering chains without crystallising them — is a consequence of exactly those properties and cannot be transferred on the strength of a ring count. The comparison is retained at Appendix C, where it belongs.

Target 7.19. (Aggregated at Target 14.2.) Decide dispersal against aggregation for units of the footprint of Corollary 7.8 in a surface of the composition of Section 6. The question belongs to the packing literature and bears on every statement of Sections 8 and 9.

8 The leaflet map, and encapsulation

Section 7 places a tethered unit in the surface. It does not say on which side of the surface the nucleic acid that unit carries lies, and at each anchor the question has a two-valued answer. The strand carries many anchors, and whether it is enclosed is a question about all of them at once. That question has a clean answer, and it is this paper's theorem.

Definition 8.1 (Anchor set and leaflet map)**.** [D] For a tethered strand s let $\mathcal{A}(s) = (a_1, \dots, a_m)$ be its anchors in strand order. A bilayer is a surface with two leaflets; let $\lambda : \mathcal{A}(s) \to \mathbb{Z}/2$ send each anchor to the leaflet of the unit carrying it, with 0 the inner leaflet. The pair $(\mathcal{A}(s), \lambda)$ is the *anchoring* of s.

Remark 8.2 (Why the leaflet and not the position)**.** [A] That a unit occupies one leaflet rather than spanning the mid-plane is Corollary 7.13, and rests there on H7; it is not assumed here. Given it, the leaflet takes two values at every anchor and is stable under any motion of the unit within its leaflet, which is the property that makes it the right datum and the anchor's position the wrong one.

Theorem 8.3 (The encapsulation condition)**.** [D] *Assume Hypothesis 7.16 and a closed surface. Then*

(a) s lies in the lumen if and only if $\lambda \equiv 0$;

(b) s lies outside the surface if and only if $\lambda \equiv 1$;

(c) otherwise s crosses the hydrophobic core, and the number of crossings is

$$c(s) = \#\{\, i < m : \lambda(a_i) \neq \lambda(a_{i+1}) \,\} = \textstyle\sum_{i<m} \big(\lambda(a_i) + \lambda(a_{i+1})\big),$$

the sum taken in $\mathbb{Z}/2$ termwise and counted in $\mathbb{Z}$.

In particular s is encapsulated if and only if λ is constant, and $c(s) = 0$ exactly then.

Proof. Let M be the mid-surface of the bilayer, a closed surface separating the two leaflets. The segment of s between consecutive anchors a_i and a_{i+1} is a path whose endpoints lie in the leaflets $\lambda(a_i)$ and $\lambda(a_{i+1})$; since M separates them, the path meets M an odd number of times when $\lambda(a_i) \neq \lambda(a_{i+1})$ and an even number otherwise, and in the second case the minimum is zero and is attained by a path remaining in that leaflet's side. Summing over i gives $c(s)$. Claims (a) and (b) follow, a strand with no crossing lying wholly on one side of M and the side being determined by the common value of λ. □

Corollary 8.4 (Encapsulation is not a metric condition)**.** [D] *Whether a strand is enclosed is a property of a $\mathbb{Z}/2$-valued function on a finite set. It is not determined by the positions of the anchors, by their spacing along the strand, by their arrangement on the surface, or by the radius of the surface, and it is invariant under every motion of the anchors within their leaflets.*

Corollary 8.5 (The cost of encapsulation)**.** [D] *Of the 2^m anchorings of a strand with m anchors, two are encapsulating, one inward and one outward. If λ is free, encapsulation is therefore a condition of $m - 1$ bits.*
That bound is the free reading, and Proposition 8.6 is the

reason it is not the operative one.

Proposition 8.6 (A sign change carries the backbone through the core)**.** [D] *At each sign change of λ the strand passes from one leaflet to the other, and by Theorem 8.3 it crosses the hydrophobic core. The segment so carried is a nucleic-acid backbone, which bears one formal negative charge per phosphate and is hydrated along its length. Burial of such a segment in an acyl core requires desolvation of the charges without compensating interaction. Taking the Born estimate for transferring a unit charge of ionic radius 2 Å from water to a medium of dielectric constant 2, the cost per phosphate is of order $40\,k_BT$, and the hydration shell carries a further contribution of the same sign [Isr11, Gen89]. A crossing buries several phosphates, so the cost of one sign change is of order $10^2\,k_BT$.*
The threshold at which the argument fails is therefore about $1\,k_BT$ per phosphate, two orders below the estimate: a compensating interaction of that strength — a counterion co-buried, a local polar defect, a protein-like sheath, none of which the architecture supplies — would return the sign changes to the free reading of Corollary 8.5. The estimate is coarse and its margin is not.

Hypothesis 8.7 (No threading)**.** [D] No anchoring forms in which λ has a sign change. Registered as H3 in Appendix A.

Corollary 8.8 (Encapsulation is one bit)**.** [D] *Under Hypothesis 8.7 and Theorem 8.3 the map λ is constant. The strand therefore lies wholly in the lumen or wholly outside the surface, and which of the two is a single bit, fixed by the side on which the strand stood when the surface closed — not the $m-1$ bits of Corollary 8.5.*

Remark 8.9 (Where the failure mode moved to)**.** [A] An earlier draft rested this section on a premise about the order of assembly — that the surface closes around an already anchored strand — and recorded that premise as the paper's dangerous one, on the ground that a threaded strand and an enclosed strand are indistinguishable in every quantity the paper computes. The premise is withdrawn at Remark D.4 and the assessment that went with it was too pessimistic.
Under Proposition 8.6 a threaded anchoring is not an alternative outcome of comparable standing; it is one whose cost grows with the number of crossings and which the assembly has no route to. What then fails, when something fails, is not that the strand threads the core but that an anchor on the wrong side does not form at all — leaving a strand anchored at some positions and free at others, with the unanchored positions in the opposite compartment.
That is a better place for the failure to sit, because it is visible. A partially anchored strand differs from a fully anchored one in the anchor count, which enters the engaged set of Section 9.3 and the capacity computed there. The earlier failure mode left no trace anywhere in the paper; this one leaves a trace in a quantity the paper already computes. Scholium 11.3 is revised accordingly.

Target 8.10. (Aggregated at Target 14.5.) Determine whether an anchor can fail to form on the compartment opposite to the strand, and what a partially anchored strand does to the engaged set. The question replaces the assembly-order target of the earlier draft and is the live form of H3.

Remark 8.11 (The echo, and its limit)**.** [A] The residue account reduces homochirality over a cluster to a parity condition on the operations relating its vessels. This paper reduces encapsulation to a parity condition on the leaflets of its anchors. The shapes agree: a $\mathbb{Z}/2$-valued datum at each site, a condition of constancy, and a failure mode invisible to every other quantity in the account.
The objects do not agree, and no common theorem is exhibited here. There the datum is the determinant of a spatial operation and is a property of a pair of vessels; here it is a leaflet index and is a property of a single anchor. A reader should take the agreement as a family resemblance among the architecture's statements rather than as a transported result, and should note that the resemblance is what one expects of an architecture whose objects are two-sided throughout — two branches at a centre, two orientations at a site, two leaflets at a surface.

9 The anchor word, and what the membrane can read

9.1 Valence, the caps, and the orientation of a unit

Definition 9.1 (The anchor word)**.** [D] A tethered strand induces a word $w(s) \in \{\mathsf{a},\mathsf{c}\}^*$ over its tethered bases, a carrying the tether T_{A} of length $\ell_{\mathsf{A}} = 10$ and c the tether T_{C} of length $\ell_{\mathsf{C}} = 13$, by Lemma 2.4. The word records the order of the letters and the gaps between them in base pairs.

Lemma 9.2 (Strand partition)**.** [A] *In a duplex exactly one strand of each base pair carries an anchor: the adenine-*

bearing strand at an A–T pair and the cytosine-bearing strand at a C–G pair. The partition of the anchor set between the two strands is therefore a function of the sequence alone.

Proof. Finite, over the four pair types; Appendix B, block V5, computed. □

Lemma 9.3 (Both units are univalent)**.** [A] *By Notation 2.3 each unit carries a nucleoside at one substituted position and a capped alkyl arm at the other. No unit is joined to two positions of the nucleic acid.*

Remark 9.4 (What the caps cost, and what they buy)**.** [A] An earlier draft of this subsection read the second arm of the cytosine unit as terminating in a free hydroxyl and the second arm of the adenine unit as carrying a second nucleoside. On that reading the adenine units were bivalent, they induced a graph on the anchor set, and the leaflet map was determined on each component of it by one value, so that λ carried a number of degrees of freedom governed by the units rather than by the strand length. That construction is withdrawn at Remark D.3. With both units univalent the graph has no edges, its components are its vertices, and the theorem built on it is vacuous.

The loss is real and is not repaired here. What the caps supply instead is of a different kind and is the subject of Proposition 9.6: both caps are apolar, so the second arm terminates in the acyl core rather than at the interface, and the unit is thereby oriented across its leaflet. The earlier reading, with a polar hydroxyl at that position, supplied no orientation at all.

Proposition 9.5 (Opposite faces)**.** [C] *The two arms of a 6,12-disubstituted unit depart toward opposite faces of the skeleton, and the conformation placing both toward one face is excluded. Imported unamended from the reaction-cell development, by way of the residue account.*

Proposition 9.6 (The unit is oriented across its leaflet)**.** [D] *Assume Proposition 9.5 and Proposition 7.1. The cap is an ethyl or isopropyl group and is apolar; the nucleoside is polar and carries the strand. The two stand on opposite faces of one skeleton. Hence in a leaflet the cap is directed toward the acyl core and the nucleoside arm toward the aqueous interface, and no disposition with the two exchanged is available.*

In particular the unit occupies one leaflet and does not span the mid-plane, so the leaflet map of Definition 8.1 is everywhere defined.

Corollary 9.7 (Remark 8.2 is derived, not supposed)**.** [D] *What Section 8 assumed of the anchoring — that each anchor occupies one leaflet and that the leaflet is the stable datum — follows from Proposition 9.6 and is not an additional premise.*

Remark 9.8 (The caps as the differentiating datum)**.** [A] The cap is where the two letters are most sharply distinguished, and the distinction is of a kind a membrane can register. Both caps sit at the same backbone depth, by Lemma 2.4, so they do not differ in how far into the core they reach. They differ in what they do at that depth: a linear ethyl terminus is compatible with the packing of the surrounding chains, a branched isopropyl terminus is not, and a branched terminus at fixed depth perturbs chain order in its neighbourhood where a linear one does not.

The magnitude of that perturbation is not computed here and is Target 9.9. What is established is that the two letters differ at the cap in shape and not merely in size, so that a reading on which the anchor alphabet is a single length scale is unavailable.

Target 9.9. (Aggregated at Target 14.7.) Determine the perturbation of chain order produced by a branched isopropyl terminus at the depth of Lemma 2.4, against a linear ethyl terminus at the same depth. The question belongs to the packing literature and fixes the acceptance windows of Section 9.3.

9.2 Orientation: the source, the frame, and the injection

The caps of Section 9.1 differentiate the two anchor types but relate no anchor to any other. This subsection supplies the relation from the datum of Definition 4.7, which is not a differentiation at all but the encoding itself.

The question is posed in information-theoretic terms because that is the form in which it has an answer, and one caution belongs with the vocabulary before it is used.

What is established below is that a certain map from sequences to surface configurations is injective, and that its fibres in the alternative branch are of computable size. Injectivity is not a communication rate: a rate presumes a decoder, and this paper exhibits none. Where the word *capacity* appears it abbreviates *the entropy of an injection*, which is what the theorems establish; Definition 9.10 fixes the abbreviation, and Remark 9.28 says what the injection is and is not evidence for.

Definition 9.10 (Capacity, as used here)**.** [D] For a map F from source words to surface configurations, the *capacity*

of F is $\log_2$ of the number of distinct configurations in its image, divided by the number of anchors. It is the entropy of the injection F induces on its fibre classes and is a property of F alone. It is not a communication rate and presumes no decoder.

The source

Definition 9.11 (The source word)**.** D For a tethered strand s let

$$W(s) = \big((\alpha_1, \beta_1), \ldots, (\alpha_m, \beta_m)\big) \in \big((\mathbb{Z}/2)^2\big)^m$$

collect the orientational data of Definition 4.7 over the anchors of s in strand order. By that definition $W(s)$ is the base-four sequence templated by those units.

Lemma 9.12 (Source entropy)**.** A *The source carries two bits per anchor. Over a sequence of m anchors there are 4^m source words, and for a sequence uniform over the four bases the entropy is exactly $2m$ bits.*

Lemma 9.13 (α is carried chemically)**.** A *α is the pair type, and by Lemma 9.2 and Notation 2.3 an anchor of one pair type bears the tether T_{A} with an ethyl cap and of the other T_{C} with an isopropyl cap. It is therefore a property of the molecule and is not lost by any motion of it, in the surface or elsewhere.*

> *Proof.* Finite, over the four pair types; Appendix B, block V6a, computed. □

Remark 9.14 (Why the chemical carriage is not a coincidence)**.** A That the pair type should happen to be legible in the tether and the cap would be a fortunate accident if the two were unrelated. They are not. By Corollary 4.4 the cap is the terminated remnant of the second bridge of the complex, severed when the substrate became a base. The molecule bears a record of its own templating because the templating is what built it.
So α is not merely correlated with the tether and cap; it is the same event seen twice. This is the strongest thing said anywhere in the paper about why a bit should survive a passage, and it is the reason the first of the two bits requires no hypothesis while the second requires H8.

Lemma 9.15 (β read against the duplex)**.** A *At a base pair exactly one strand carries the anchor, by Lemma 9.2. Which of the two it is distinguishes the two bases of that pair type, and is therefore β read against the duplex rather than against the cluster's frame. The two readings agree at every anchor: a frame that orients the segment orients its strands.*

Lemma 9.16 (The strand orders the anchors)**.** A *The anchors of a strand are held in sequence by the strand itself, at positions $1, \ldots, m$ along the segment. The order is a property of the covalent backbone and is preserved under every motion of the surface, the anchors being carried by the strand and not by the surface.*
In consequence the surface state is an ordered word and not a multiset: the position number of an anchor is available wherever the anchor is, and it is what makes the anchors a sequence in the surface rather than a population.

Remark 9.17 (What the ordering is worth)**.** A This deserves explicit statement: it is the only element of this section that costs no premise, and it is easily mistaken for bookkeeping.
Were the ordering lost, the surface would hold the base composition of the segment and nothing more: the fibres of the map would be multinomial in m rather than uniform, and at twelve anchors the largest would exceed three hundred thousand words against the four thousand of the slaved-face reading (block V6d). The strand is what prevents this, and it prevents it for a reason that has nothing to do with the membrane — a covalent backbone does not permute its own residues.
So the mapping of a sequence into a surface is carried by two things of quite different kinds: the letters by orientation, which is a premise, and the order by covalency, which is not.

Remark 9.18 (Which bit is at risk)**.** A Lemma 9.13 settles half the source and leaves the other half entirely open. The two halves behave differently for reasons that should be set out.
α is intrinsic. It was fixed by the templating and it was written into the molecule as a tether and a cap, so it accompanies the unit wherever the unit goes and no premise of this paper bears on it.
β is frame-relative. It records an orientation, and an orientation is a relation to a frame. The frame in which it was fixed — that of the cluster, common to all its units — does not accompany the unit into the surface. So β survives only if the surface supplies a frame of its own, and only if the unit's orientation in that frame is free to record it. Sections 9.2.2

and 9.2.3 take these in turn.

The frame

Definition 9.19 (The surface frame)**.** [D] By Proposition 9.5 the skeleton has two faces. Let $\sigma : \mathcal{A}(s) \to \mathbb{Z}/2$ record which face a unit presents away from the bilayer mid-plane, and let λ be the leaflet map of Definition 8.1.

Proposition 9.20 (The normal replaces the stack)**.** [D] *A closed surface possesses a globally defined outward direction. The question which face is presented away from the mid-plane is therefore one and the same question at every anchor of the surface, and σ is a function on $\mathcal{A}(s)$ referred to a single frame.*
This is the condition under which the anchors encode collectively rather than severally. Were the available frame local, each anchor would carry a bit referred to its own neighbourhood, no pattern over anchors would be defined, and the sequence would not be present in the surface in any sense. The bilayer normal supplies globally what the stack supplied in the cluster, and it is the only datum of a fluid surface that does: positions diffuse, neighbours exchange, and orientations relative to the normal do neither.

The injection, and the premise it turns on

Remark 9.21 (A derivation withdrawn)**.** [A] An earlier draft derived an identity $\sigma = \omega + \lambda$, where ω records which substituted position is directed at the interface, from the requirement that the nucleoside arm reach the interface and the cap the core. The derivation assumed that the arm is rigidly assigned to the face of the substituted position bearing it, so that fixing which position points outward fixes which face is presented.
The assumption is not available. The arm is a phosphodiester of nine backbone atoms and is flexible over its length, by the same token that Hypothesis 7.11 requires it to fold; an arm that can fold back into the core can also reach the interface from either face of the skeleton. The identity is withdrawn at Remark D.7.
The cost of the withdrawal should be stated, since it constitutes the substance of this subsection rather than an incidental repair. Under the identity, σ was a function of ω and λ, hence of α alone under encapsulation; the surface could then hold one bit per anchor and the polarity of every pair was lost. The withdrawal is what permits σ to carry β.

Hypothesis 9.22 (Face freedom)**.** [D] The flexible nucleoside arm permits a unit to present either face while delivering its nucleoside to the interface; σ is therefore not determined by ω and λ. Registered as H8 in Appendix A.

Theorem 9.23 (The map is injective under face freedom)**.** [D] *Assume Hypothesis 9.22, Hypothesis 8.7 and Proposition 9.20. Then the map*

$$W(s) \longmapsto \big(\omega(a_i), \sigma(a_i)\big)_{i=1}^{m}$$

carrying a source word to the surface state of its anchors is injective, with $\omega = \alpha$ by Lemma 9.13 and $\sigma = \beta + c$ for a constant $c \in \mathbb{Z}/2$ fixed by the leaflet. The surface therefore holds two bits per anchor and the base-four word transfers entire, with no kernel.

Proof. $\omega = \alpha$ is Lemma 9.13. Under Hypothesis 9.22 σ is free of ω, and by Proposition 9.20 it is referred to one frame across the surface, so it may take the value β shifted by the single global constant relating that frame to the cluster's. Under Hypothesis 8.7 λ is constant by Corollary 8.8, so c is one constant and not one per anchor. The pair (ω, σ) then determines (α, β) at each anchor, and injectivity over the word follows. Appendix B, block V6b, computed at four word lengths. □

Theorem 9.24 (The fibre dichotomy)**.** [A] *The map of Theorem 9.23 has fibres of exactly one of two sizes.*

(i) Under Hypothesis 9.22: two bits per anchor, the map of Theorem 9.23 a bijection, and no loss.

(ii) Without it, σ being slaved to ω and λ: one bit per anchor. The fibres of the map have size 2^m, and what is lost is exactly β at every anchor — which pairs are of which type is retained, and which strand of each pair carries the anchor is not.

Proof. Finite, by enumeration over base-four words; Appendix B, blocks V6b and V6d, computed. The fibres are of size 1 in case (i) and uniformly of size 2^m in case (ii); in both the ordering of Lemma 9.16 is in force, and block V6d prices it by exhibiting the multinomial fibres that would obtain without it. □

Corollary 9.25 (Encapsulation is congruence of two patterns)**.** [D] *Under Theorem 9.23, λ is constant if and only if $\sigma = \beta + c$ for a single constant, that is if and only if the face pattern presented by the units agrees with the orientational half of the source word up to one global flip. Each sign change of λ appears as a discrepancy between the two patterns at every anchor past the crossing.*

Remark 9.26 (What this establishes, and in what sense)**.** [A] The result is that a surface assembled from unrecruited units of a family can hold the entire base-four sequence that the recruited units of the same family templated, at two bits per anchor and with no kernel, under one premise about the flexibility of an arm.
Three qualifications belong with it and none is a formality. The anchors hold the sequence; nothing in this paper reads it, acts on it, or recovers it, and Scholium 9.30 is at pains about the difference. The premise is undischarged and the alternative branch costs exactly half. And the encoding that transfers is the encoding of the templating orientations, which is the sequence only because Definition 4.7 makes it so — a reader who denies that identification denies the source, not the channel.

Remark 9.27 (The limitation the marker inherits)**.** [C] The residue account records that an orientation marker registers which of two orientations a unit is in and not how the two are related in space, and that no statement about the pattern can see a determinant. That limitation is inherited here unamended and bounds what this subsection claims.
σ and ω are such markers. They carry the letters of Definition 4.7 and they fix nothing about the spatial relation between two units — not the parity of the operation carrying one to another, not the handedness of anything, and not the geometry of any stacking between them. Remark 13.4 states what the two papers together say about this, which is that a marker cannot carry a determinant and can carry a letter.

Remark 9.28 (On the absence of a decoder, and what it does and does not mean)**.** [A] This paper exhibits no process that reads the configuration Theorem 9.23 establishes. That is a limit on what the paper claims and it should not be mistaken for a claim about what is possible.
Two things follow positively from the injection, and they are the reason the result is worth establishing at all rather than merely worth qualifying.
First, injectivity is the *necessary* condition on any decoding whatever. A map with non-trivial fibres cannot be inverted by any mechanism, however ingenious; a map without them can be inverted in principle, and what remains is to find a mechanism that does. Theorem 9.24 therefore separates the case in which a decoding principle could exist from the case in which it could not, and finds the architecture in the first under Hypothesis 9.22. The paper establishes necessity and is silent on sufficiency; it does not assert that sufficiency fails.
Second, the architecture supplies a physical path along which such a mechanism would have to run, and supplies it as a by-product of the templating rather than as an addition. The tether is a covalent route from a unit embedded in the membrane to a base of the nucleic acid. A perturbation at the membrane — a change in local order, in curvature, in the packing about a cap — is therefore not isolated from the sequence by any gap that would have to be bridged; it is one molecule away from it. Whether such a perturbation propagates, in what direction, and with what specificity, is not addressed here and is Target 9.29. What can be said is that the tethering complex is a candidate skeletal framework for a decoding principle, and that a corpus intending to look for one would look here.

Target 9.29. (Aggregated at Target 14.11.) Determine whether a perturbation of the membrane propagates along the tether to the nucleic acid, and whether the reverse path carries. Signalling and modulation between the enclosure and the sequence it encloses are not addressed in this paper and are proposed as a subject of future study; the injection of Theorem 9.23 is the precondition such a study would need and the tethering complex is the structure along which it would run.

Scholium 9.30 (What "the encoding reaches the membrane" means here)**.** The phrase is the one this section is most likely to be summarised by, and it carries less than it sounds like and more than the earlier draft allowed.
Less, in that what is established is a state and not a use. The units in the surface stand in definite orientations; the pattern of those orientations is the base-four word, up to a global flip; and that is a statement about the configuration of a surface. It is not a statement that anything in the surface reads the pattern, that the pattern has a consequence for what the surface does, or that it is recoverable by any process the corpus presently describes.
Remark 9.28 says what that does and does not leave open. In short: the paper establishes the condition without which no decoding could occur, and does not establish one that does. It does not assert that none can be built, and it identifies the tethering complex as the structure along which one would run.
More, in that the pattern is not a copy of the sequence but the sequence's own template orientations, carried by the objects that held them. The surface does not receive a transcription. It receives the templates, arranged.

Target 9.31. (Aggregated at Target 14.3.) Determine whether the nucleoside arm permits a unit to present either face while reaching the interface. It is H8, and by Theorem 9.24 it decides whether the surface holds the whole

base-four word or half of it.

9.3 The helical filter, and the metric channel

Remark 9.32 (The weaker and the more robust of the two channels)**.** [A] What follows treats the length and cap differences of Lemma 2.4 as a second channel. It is weaker than the orientation channel of Section 9.2 in every respect: its data are metric rather than $\mathbb{Z}/2$-valued, its acceptance windows are not computed here, its map has a kernel, and it reaches only anchors in helical phase.
It is retained for two reasons. It is independent of Hypothesis 9.22, so it survives the branch of Theorem 9.24 on which the orientation channel loses half its capacity. And it carries α by a second route: the tether length and the cap are both properties of the pair type, so a surface that could resolve either would recover what Lemma 9.13 already guarantees chemically. The channel is therefore redundant where it works and is not the paper's route to anything.

Theorem 9.33 (The helical-phase filter)**.** [D] *Let a duplex lie against the surface with helical repeat p base pairs, and let the azimuth of anchor i be $\phi(i) = 2\pi i/p$ modulo 2π. An anchor engages the surface only if $\phi(i)$ lies in an acceptance window W_ℓ determined by its tether length ℓ. The engaged set is*

$$\mathcal{E}(s) = \{\, i : \phi(i) \in W_{\ell(i)} \,\},$$

and $W_{\ell_A} \neq W_{\ell_C}$, the longer tether admitting the wider window.

Remark 9.34 (What the filter does not touch)**.** [A] Engagement in the sense of Theorem 9.33 is a metric condition on reaching the surface from a given azimuth. It is not a condition on being anchored: an anchor that has formed holds its unit in a leaflet whatever the azimuth, and Theorem 9.23 is stated of anchors and not of engaged anchors.
The distinction is worth making because the two channels would otherwise appear to compete. They do not. The orientation channel reports the state of every anchored unit; the metric channel reports which anchors a surface could resolve by tether reach. A filter on the second leaves the first untouched.

Theorem 9.35 (Capacity of the metric channel)**.** [D] *Write $e = |\mathcal{E}(s)|$ for the number of anchors in phase. The map $s \mapsto \mathcal{E}(s)$ is not injective: its fibres are of size*

$$4^{m-e} \cdot 2^{e},$$

and the information retained is e bits, one for each engaged anchor and none for the rest.

> *Proof.* The channel's only per-anchor datum is the pair type, by Lemma 2.4: the tether length and the cap both report α, and the polarity β has no metric carrier. An engaged anchor therefore distinguishes two letters of four and contributes a factor 2 to the fibre; an anchor out of phase reports nothing and contributes 4. Multiplying over the m anchors gives the displayed size, and the retained information is $\log_2(4^m/(4^{m-e}2^e)) = e$ bits. Appendix B, block V6e, computed at several engagement fractions. □

Corollary 9.36 (The windows fix the engagement and not the report)**.** [A] *The acceptance windows of Theorem 9.33 enter the capacity only through e. What an engaged anchor reports is fixed by Lemma 2.4 and is one bit whatever the windows are, so Theorem 9.35 is complete as it stands and Target 14.7 supplies a value for e rather than a missing term.*

Remark 9.37 (The two channels compared, with both capacities in hand)**.** [A] The comparison can now be made exactly. The orientation channel carries $2m$ bits under Hypothesis 9.22 and m without it (Theorem 9.24). The metric channel carries e bits, $e \le m$, and carries the same bit the orientation channel carries first — the pair type — so the two are not additive.
Their union carries $2m$ bits under Hypothesis 9.22 and $\max(m, e) = m$ without it. The metric channel therefore adds nothing to the capacity in either branch. What it adds is redundancy in the second: the pair types are then reported twice, by chemistry through the orientation channel and by reach through this one, and a result established twice is established differently from one established once.

Corollary 9.38 (What survives fluidity here)**.** [D] *What this channel delivers is the gap composition between consecutive engaged anchors, which is invariant under any motion of the surface preserving strand order, and not an arrangement of anchor positions, which is not. This is why Proposition 3.1(iv) refuses the spatial reading for the metric channel as it does for the orientational one.*

Scholium 9.39 (Why the weaker channel is kept)**.** A paper may drop a channel that carries nothing its stronger channel does not. This one is kept because the two fail differently, and a reader deciding what to believe should see both failure surfaces.
The orientation channel carries two bits or one according to

Hypothesis 9.22, a conformational premise about an arm. The metric channel carries at most one bit and requires acceptance windows not yet computed, but it requires nothing of the arm. Should Hypothesis 9.22 fail, the account is left with one bit per anchor by two independent routes rather than by one, and the pair types are then established rather than merely unrefuted.

That is a modest thing to have and it is stated modestly. The section computes its resolution exactly — e bits for e engaged anchors, by Theorem 9.35 — and what the uncomputed windows withhold is the value of e, not a term of the formula.

A fair objection is that redundancy on a bit which Lemma 9.13 calls unconditional protects against nothing. The answer names what the unconditionality assumes. Lemma 9.13 holds while the tether and the cap are intact, and it is exactly a hydrolysis at the cap, an exchange of the terminal group, or a severance of the arm that would lose α while leaving the unit in the surface. The metric channel reports the length of the *remaining* arm, which such an event changes rather than erases. So the redundancy is not against the failure of a premise but against the chemical degradation of a molecule, which is a different hazard and one the architecture gives no reason to exclude over the lifetime of an enclosure.

That is the whole of the case for keeping the section, and it is a narrow one. A reader who is untroubled by degradation may treat Section 9.3 as a remark.

10 Closure, and the stoichiometric bound

Definition 10.1 (Closure)**.** [D] A closed bilayer vesicle of radius R whose lipids present head-group area a carries

$$N(R) \;=\; \frac{2\cdot 4\pi R^2}{a}$$

molecules, the factor two counting both leaflets.

Proposition 10.2 (Lipids per vesicle)**.** [A] *On route A one lipid is produced per dimer and one dimer consists of two vessels, so the yield is one half of a lipid per unrecruited vessel.*

Definition 10.3 (The two confinement models)**.** [D] Write $L = hn$ for the contour length of a duplex of n base pairs, h the rise per base pair, and L_p its persistence length. Two conditions on R are considered.

Model 1, free in the lumen. The strand is unattached and occupies the interior as a wormlike coil; R is required to admit its radius of gyration, $R^2 \geq L_p L/3$ for $L \gg L_p$.

Model 2, anchored to the inner leaflet. The strand lies against the inner surface and follows its curvature; the bending energy $k_B T L_p L/2R^2$ is required not to exceed a tolerance E^*, whence $R^2 \geq L_p L/2E^*$.

Remark 10.4 (Model 2 is this paper's case)**.** [A] The distinction is not a matter of which idealisation is more convenient. By Section 8 the strand of this paper is anchored at every tethered position and lies against the inner leaflet; it is not free in the lumen, and model 1 describes a different object. The difference is large and runs in the helpful direction. A coil must be *contained*, which costs a volume; a surface-laid duplex must only be *bent*, which costs a curvature. At a thousand base pairs the first requires a vesicle of some seventy-five nanometres and the second of some thirty, and the lipid count falls with the square. Anchoring, which Section 8 introduces for the sake of encapsulation, pays for part of the enclosure it requires.

Theorem 10.5 (The pool ratio is independent of the strand length)**.** [D] *Let $\nu(n)$ be the number of unrecruited vessels required per encoded vessel to close a surface about a strand of n base pairs, an encoded cluster being taken at one vessel per base pair. Then in both models of Definition 10.3 R^2 is proportional to n, hence N is proportional to n, and ν is constant in n:*

$$\nu_1 = \frac{16\pi L_p h}{3a}, \qquad \nu_2 = \frac{8\pi L_p h}{aE^*}.$$

Proof. By Definition 10.3, $R^2 = cL_p hn$ with $c = \frac{1}{3}$ or $c = 1/2E^*$. By Definition 10.1, $N = 8\pi R^2/a$, and by Proposition 10.2 the vessels required are $2N$. Dividing by n removes the dependence and leaves the displayed constants. Appendix B, block V7, computed at six strand lengths in both models. □

Corollary 10.6 (The number)**.** [D] *At $L_p = 50$ nm, $h = 0.34$ nm, $a = 0.65$ nm^2 and $E^* = 10\,k_B T$, $\nu_2 \approx 66$ and $\nu_1 \approx 438$. The architecture therefore requires an unrecruited pool of order 10^2 vessels per encoded vessel, and not more, however long the sequence enclosed. The figure carries a stipulation: E^* is set by the author and not measured, and over the range swept at block V7b it moves ν_2 between 22 and 219. What does not move with it is the constancy of ν in n, which is Theorem 10.5 and turns on $R^2 \propto n$ alone. The figure is computed for a bilayer of the route-A lipid, which the dominant substrate supplies; the minority substrate*

contributes a spanning species rather than a second phase, and Proposition 10.2 counts only the former.

Proof. Finite; Appendix B, blocks V7 and V7b, computed with a sensitivity sweep. □

Remark 10.7 (What is omitted, and which way each omission runs)**.** [A] The model is coarse and a reader is owed the direction of each thing left out of it, since a bound whose errors all run one way is not a bound.
Raising ν: the poly-adenosine–chrysene initialiser, which occupies lumen the model does not charge for; the electrostatic cost of confining a polyanion with its counterions, which is nowhere in the bending term; and any excess of R over its floor, which enters as R^2.
Lowering ν: the tethered units themselves, which occupy leaflet area and so displace unrecruited lipid one for one by their own footprint. By Corollary 7.8 that footprint is 0.39 to 0.43 nm^2 against a head-group area of 0.65, so each anchored unit displaces about six tenths of a lipid. The table does not credit this and the figures therefore overstate the requirement.
Of unknown sign: the head-group area of a dialkyl phosphate diester, which is taken at a literature value for the class rather than computed for this lipid, and the bending tolerance E^*, which is a stipulation and not a measurement. Block V7b sweeps both, and ν_2 moves between roughly twenty and roughly two hundred over the plausible range. The order survives; the figure does not.

Scholium 10.8 (The sentence this replaces)**.** An account of this kind is liable to be summarised as producing a prototype cell from its own materials, and the summary should be tested against the count before anyone else tests it.
What the count returns is a condition on the setting rather than a product of the architecture: an enclosure is available where the unrecruited pool exceeds the encoded cluster by a factor of order a hundred. That is a requirement, and it is a mild one — mild because it does not grow, by Theorem 10.5. An architecture whose pool requirement scaled with the length of the sequence would enclose short strands and nothing else, and would be an argument against itself at any interesting length. This one encloses a strand of thirty thousand base pairs on the same terms as one of three hundred.
That is the strongest form the closure claim takes, and it is weaker than the summary it replaces in one respect and stronger in another. It does not say the architecture supplies its own enclosure; it says what a setting must supply. But it says so with a number that does not deteriorate, which is more than the earlier framing offered.

11 Consolidated register

This section states, in one place, what the account answers and on what. It adds nothing. Its purpose is that a reader who has followed the argument should be able to see which answers are finite, which rest on a supposition, and which are open.

11.1 What is answered, and on what

Can the unrecruited dimer yield a bilayer-forming lipid?
Yes, by route A on the dominant singly bridged substrate, alone of four admissible routes. The selection within the diacyl class is by tail length and not by topology.
Rests on: Finite, over the cut sets (Thm. 5.10, Cor. 5.16).
Standing: [A] Computed, blocks V1, V2, V2b.

What does the minority substrate contribute?
A macrocyclic bolaamphiphile of twenty-eight ring carbons with two pendant tails of eight, spanning about fifteen Å between its two polar centres: a species of the topology that staples the leaflets of a bilayer.
Rests on: Finite (Cor. 5.12, Cor. 5.13).
Standing: [A] Computed, block V2b. Whether it is accommodated, and at what mole fraction, is open (Target 14.4).

Does the composition agree with a reference phospholipid?
In carbon it does, but the total is not the informative quantity. The partition, four in the linker and thirty-six in two tails, is a dialkyl phosphate diester and not a phosphatidylcholine.
Rests on: Finite (Thm. 6.4); O, N and H are placed, not counted (Conv. 6.1).
Standing: [A] Computed, blocks V3 and V4; an audit and not evidence.

Where does the tail's unsaturation lie?
At Δ9, the ether at C6 standing at carbon ten of eighteen under both admissible cut sets; the product is a di-*O*-(octadec-9-enyl) phosphate.
Rests on: Finite (Thm. 5.20, Cor. 5.21).
Standing: [A] Computed, blocks V2c and V3b. The geometry of the double bond is not fixed (Target 5.25).

Where does the head group come from?
From outside the dimer: one nitrogen, which the architecture admits, and four carbons, which the budget does not hold.
Rests on: Sup. 6.7, H1.
Standing: [D] Supposed where used. The bilayer does not rest on it (Cor. 6.6).

Does the tethered unit sit in the surface?
By topology yes. The orientation is a tilt range and not a direction; over it the footprint is 0.39 to 0.43 nm^2 and the depth fifty-two to seventy-two per cent of a leaflet. No resemblance to a sterol is used.
Rests on: Prop. 7.1, Prop. 7.6, Cor. 7.8.

Standing: [D] Geometry computed, block V8; the regime is undecided (Target 7.19).

Does it lie within one leaflet?
Only if the capped arm folds, by 2.8 to 5.5 Å of its eleven. Fully extended the unit is 30 to 33 Å against a 27 Å core.
Rests on: Hyp. 7.11, H7.
Standing: [D] Supposed. The premise on which the leaflet map is defined at all (Target 7.15).

When is an anchored strand enclosed?
Exactly when the leaflet map is constant; otherwise it crosses the core once at each sign change.
Rests on: Thm. 8.3, under H2 and H7.
Standing: [D] Established. The condition is not metric (Cor. 8.4).

Is the leaflet map constant?
Yes, unless the backbone threads the hydrophobic core, whose cost grows with the number of crossings.
Rests on: Prop. 8.6, H3.
Standing: [D] Derived under H3; the live question is partial anchoring (Target 8.10).

Does the sequence reach the surface?
Yes, as a pattern of unit orientations: the sequence fixes which substituted position bears the nucleoside, and that fixes the face each unit presents.
Rests on: Thm. 9.23, under H8.
Standing: [D] Established given H8; the metric channel of Section 9.3 is separate and weaker.

How much of it reaches the surface?
One bit per anchor, with no kernel, under encapsulation.
Rests on: Thm. 9.24.
Standing: [D] Computed, block V6b; contingent on H8 by Thm. 9.24.

What decides whether the strand is inside?
The face pattern agreeing with the anchor word up to a global flip.
Rests on: Cor. 9.25.
Standing: [D] Established; equivalent to constancy of the leaflet map.

Can any sequence be encapsulated?
Not settled. If the surface constrains the presented face, only single-letter anchor words can; if not, any can.
Rests on: Thm. 9.24, H8.
Standing: [D] Open, and the paper's sharpest falsifiable consequence (Target 9.31).

Does anything of it survive lateral diffusion?
The orientation pattern does, being $\mathbb{Z}/2$-valued at each anchor and carried in strand order; no arrangement of positions does.
Rests on: Thm. 9.23; Cor. 9.38 for the metric channel.
Standing: [D] Established, and it is a limitation of the surface rather than of the encoding.

Can the pool close a surface about a strand?
Only if it exceeds the cluster by a factor ν of order 10^2.
Rests on: Thm. 10.5, Cor. 10.6, H5.
Standing: [D] Computed given the geometry; the geometry is supposed.

Does that requirement grow with the sequence enclosed?
No. R^2 is proportional to n in both confinement models, so ν is constant in n.
Rests on: Thm. 10.5.
Standing: [D] Established; the constant differs between the models by a factor of about seven.

Is a cell produced?
No. A closed surface containing a strand is not a cell, and nothing here bears on metabolism, division, transport or replication.
Rests on: —
Standing: [A] Refused at Prop. 3.1(i), before every construction.

11.2 How much is finite

Remark 11.1 (The four kinds, counted)**.** [A] Of the seventeen entries above, four are finite computations over the record and stand whatever becomes of any hypothesis: the scission classification, the product of the minority substrate, the carbon partition, and the position of the retained unsaturation with the formula it yields. Eleven are derived under named premises, of which two are suppositions in substance — the head group and the containment of the unit within one leaflet — and one is open, being the fibre dichotomy. One is a refusal. Four, eleven, one and one make seventeen.
A fifth computation sits inside a derived entry and should be counted where it belongs: the skeleton geometry of block V8 is finite, and what rests on a premise is not the geometry but the siting, that a unit so shaped occupies a leaflet in the way Section 7 says. A reader who denies every hypothesis of this paper keeps five blocks of arithmetic and loses every sentence about a membrane.

Remark 11.2 (Where the premises are concentrated)**.** [A] The distribution merits comment because it runs against the shape of the subject, and in the same direction the residue account records for its own.
Membrane arguments are usually thermodynamic throughout: a packing parameter, a phase diagram, a free energy of transfer. Here the thermodynamic content is confined to four premises — that units disperse rather than aggregate (H2), that a charged backbone does not thread an acyl core (H3), that a capped arm folds rather than extends (H7), and that the nucleoside arm permits either face to be presented (H8) — and everything else is a finite check over a graph, a $\mathbb{Z}/2$ identity, or a scaling argument.
That is a virtue for auditability and a liability for confidence.

> The finite parts cannot be wrong in a way that inspection would not catch. The four premises cannot be checked by inspection at all, and three of the four are stated here without a calculation behind them.

11.3 What the account would look like at each failure

H1, the head group. The letter and nothing else. The lipid reverts from a phosphatidylcholine to the dialkyl phosphate diester of Theorem 6.4, which is lamellar as it stands, and every statement of Sections 7 to 10 is untouched. This is the cheapest failure in the register and Corollary 6.6 is why.

H2, the dispersed regime. The subject. Under aggregation the units form a domain rather than a solution; the anchors of a strand are not independently placed; the leaflet map is evaluated at a boundary; and the orientation relation is stated of units whose faces contact one another rather than the core. Sections 5, 6 and the geometry of Section 7 survive, being about cut sets, counts and one unit. Sections 8 to 9 do not.

H3, no threading. Encapsulation returns from the one bit of Corollary 8.8 to the $m - 1$ bits of Corollary 8.5, and a strand may be transmembrane. Theorem 8.3 itself is unaffected, being the condition and not its satisfaction. The live form of the failure is partial anchoring, which the anchor count registers (Remark 8.9).

H4, the helical windows. Section 9.3 only. The orientation channel is independent of it and carries the whole anchor word regardless.

H5, the closure geometry. The value of ν and not its constancy. Theorem 10.5 turns on $R^2 \propto n$, which no parameter value disturbs; what is lost is the figure of order 10^2, and the requirement on the pool becomes unquantified rather than false.

H6, the record. The audit value of blocks V0 to V5, and the identification of the imported objects with the corpus's. The architectural statements are about cut sets on a graph and survive a defect in the record they run over — though a defect there is to be reported as a defect, not reconciled.

H7, the folded arm. The most expensive failure in the register. The unit spans the bilayer, λ is not a function on anchors, Theorem 8.3 has no subject, Theorem 9.23 loses the term it is stated in, and Sections 8 to 9.2 are about an object that does not exist. Sections 5, 6, the geometry of Section 7 and the closure arithmetic of Section 10 survive.

H8, the presented face. Exactly half the channel, and no more. The source of two bits per anchor is unaffected, and so is the chemical carriage of the first of them: by Lemma 9.13 the pair type is written into the tether and the cap and is lost by no motion. What fails is the carriage of the second. With the presented face slaved to the tether type, σ is a function of α under encapsulation, β has no carrier, and by Theorem 9.24(ii) the fibres of the channel acquire size 2^m: the surface retains which pairs are A–T and which C–G, and loses which strand of each carries the anchor.

The account is not thereby left without a channel, contrary to what an earlier draft supposed. It is left with one bit per anchor, by two independent routes — the orientation of Section 9.2 and the metric channel of Section 9.3, which is independent of this premise — and with the ordering of Lemma 9.16, which costs no premise at all.

> **Scholium 11.3** (The asymmetry of the table)**.** Most failures above cost a statement and leave a smaller account that is still an account. H1 costs a letter; H4 costs a section; H5 costs a figure. The question worth putting is whether any failure leaves the account intact and the conclusion false — the shape the residue account records at its H7, and the shape an earlier draft of this paper attributed to its own H3. The answer must distinguish two things an earlier draft ran together: whether a failure is *stated* by the account, and whether it is *detectable* by anyone.
>
> Stated, all of them are. H3 failing costs the anchor count. H2 and H7 failing remove the subject. H8 failing halves the fibre resolution, and Theorem 9.24 prints both branches.
>
> Detectable, none of them is, and the draft that implied otherwise was wrong. The account has no observation that discriminates its branches — not the capacity branches, and not, as the next paragraph records, which compartment the strand occupies. Printing both branches is not the same as being able to tell which obtains; it is the difference between a theory that conceals its alternatives and one that does not, which is a virtue of exposition and not of evidence.
>
> So what the paper holds is this. No failure leaves the account silently intact, because the account names every branch it cannot choose between. Every failure leaves it undecided, because it has no measurement. That is weaker than the earlier draft claimed and stronger than nothing, and it is the honest form.

12 Falsification register

Each entry names what would refute the statement, and only what would. Where a statement is refuted with another and not independently, that is said rather than an entry invented for it.

Lemma 5.3
An edge inventory for X other than eighteen cycle edges and three chords, which would move the cyclomatic number and with it the forced cut count.

Lemma 5.5, Theorem 5.6
A recount at block V1 disagreeing at any row; or a chain-forming cut set terminally attached at both substituted positions, which Theorem 5.6 excludes on the ground that C6 and C12 are not cycle-adjacent.

Proposition 5.8, Theorem 5.10

A recount at block V2 disagreeing; a fifth admissible route; or a route reaching the diacyl topology at tails in the lamellar range from a cut set other than A, which would remove the selection of Corollary 5.16.

Corollary 5.12, Corollary 5.13
A macrocycle of other than twenty-eight ring carbons or other than fourteen between the phosphorus centres; a bolaamphiphile of this arc length forming a bilayer rather than a monolayer; or a demonstration that the macrocyclic form is dominant rather than minority, which would exchange the roles of the two channels and return the account to the monolayer.

Theorem 5.20, Corollary 5.21
An elimination reaching a position other than Δ9 or Δ10, which the single ether carbon with two chain neighbours forbids; or a product formula at block V3b disagreeing with the construction.

Proposition 5.19
A degree-of-unsaturation count for the skeleton other than thirteen; or a ring discharge other than the four of Lemma 5.3.

Theorem 6.4
A recount at blocks V3 or V4 disagreeing; a generator adding carbon to the dimer, which would free the partition; or a dialkyl phosphate diester of this partition that is not lamellar.

Supposition 6.7
A route to a quaternary head group from the dimer alone, which would refute the supposition by making it unnecessary rather than false, and would strengthen the account.

Proposition 7.3, Lemma 7.4
An embedding recovering other than eighteen carbons, which would show the lattice construction is not of this skeleton; or a locant assignment consistent with the chord pattern and placing C6 or C12 other than on an interior ring.

Proposition 7.6, Corollary 7.8
A disposition giving the two substituted positions no depth separation, which would leave one arm unable to reach the interface — on the present embedding that is the single tilt $\phi = 43.9^{\circ}$, so the proposition is refuted by showing the normal confined to it; or a footprint outside the range of the sweep at block V8; or a folded extent for the capped arm above 5.9 Å, which would empty the range of Corollary 7.8 from the shallow end.

Hypothesis 7.11, Corollary 7.13
A capped arm extending rather than folding, so that the unit spans the bilayer. This is the most expensive refutation available against the paper and is entered at Target 7.15.

Proposition 7.1
A partition coefficient placing the tethered unit in the aqueous phase; or a phosphodiester geometry placing the polar group in the core.

Hypothesis 7.16
An aggregation of tethered units into a domain at the stated surface composition, which replaces the object of Sections 8 and 9 rather than weakening their statements.

Theorem 8.3
An anchored strand with non-constant leaflet map that is nonetheless enclosed; or an anchor occupying neither leaflet, which Corollary 7.13 excludes and which would have to be argued against it.

Corollary 8.4
Falsified with Theorem 8.3 and not independently.

Proposition 8.6, Corollary 8.8
An anchoring exhibited with a sign change of λ; or a backbone segment buried in an acyl core at a cost the proposition's estimate does not reach, which would return encapsulation to the $m - 1$ bits of Corollary 8.5.

Proposition 9.6
A cap residing at the interface rather than in the core; or a unit disposition with cap and nucleoside arm exchanged, which would return Remark 8.2 to the status of a premise.

Lemma 9.2
A pair type carrying an anchor on both strands, or on neither; or a tether at a base other than adenine and cytosine, which the patent record would then be wrong to have figured.

Lemma 2.4
A backbone count at block V5 disagreeing; or a cap other than ethyl and isopropyl, which would move the differentiation of Remark 9.8 without disturbing the orientation relation.

Theorem 9.23
A unit disposed with its cap at the interface and its nucleoside arm in the core, which would refute Proposition 9.6 and with it the identity; or an anchor type laying its tether along the same sense as the other, which would make ω constant and the relation vacuous.

Corollary 9.25, Theorem 9.24
An encapsulated strand whose face pattern is not congruent to its anchor word, which would refute the identity or the encapsulation condition.

Theorem 9.24, Hypothesis 9.22
One exhibited encapsulated strand of non-constant anchor word decides for case (a); a surface admitting only one presented face decides for case (b) and bounds the architecture to single-letter words. The proposition itself is refuted only by a third value of σ, which $\mathbb{Z}/2$ does not admit.

Theorem 9.33, Theorem 9.35
An acceptance window admitting every azimuth, which would make the filter trivial; a duplex conformation with no fixed repeat; or a recomputation giving injectivity, which would refute Scholium 9.39 in the favourable direction.

Lemma 9.16
An anchoring in which the surface reorders the anchors of a strand, which would require the backbone to permute its residues.

Theorem 10.5, Corollary 10.6
A confinement condition on R not proportional to n, under which ν would cease to be constant and the closure claim would deteriorate with strand length; a lipid-per-vessel count other than Proposition 10.2 gives; or a head-group area outside the range swept at block V7b.

Remark 10.4
A reason the anchored strand must be treated as a free coil after all, which would restore the volume constraint and raise ν about sevenfold.

13 Precedence

Ruling 13.1 (Disposition against the coordinating paper)**.** [A] *Consistent, extending. The status labels, the locant ruling and the four-level convention separating connectivity, chemical admissibility, geometric accessibility and physical realization are adopted here unamended, and no statement of that paper is superseded or qualified. This paper adds a branch to the arc it coordinates and nothing to its coordination.*

Ruling 13.2 (Disposition against the structure development)**.** [C] *Consistent; one use added. The vessel graph with its eighteen-cycle and three chords, and the locant registry on it, are imported and are the object on which every cut set of Section 5 is defined. That development classifies retained subgraphs; this one classifies cut sets on the same graph, and the two classifications are over different objects and do not meet.*

Ruling 13.3 (Disposition against the residue account)**.** [A] *Consistent; two consequences added, neither amending it. First, the edge* C5–C6*, which that account severs at sixteen of its nineteen rows, is the locus at which elimination here fixes the unsaturation of the tail at* Δ9 *(Theorem 5.20, Remark 5.22). That is a fact about the skeleton and about where the two branches of the arc act; it establishes no relation between the operations and none is claimed.*
Second, the statement that the two arms of a unit depart toward opposite faces, which that account imports for its own purposes, carries here the orientation of a unit in a leaflet (Propositions 9.5, 9.6) and through it the identity of Theorem 9.23. The statement is used unamended and its own consequences there are untouched.

Remark 13.4 (A coordination finding: what a marker can and cannot carry)**.** [A] The residue account records that an orientation marker registers which of two orientations a unit occupies and not how two orientations are related in space, and that no statement about the pattern of markers can see a determinant. It records this as a limitation, and it is one: the handedness of an assembly is not recoverable from its orientation pattern, and that is why the parity of the assembly relations had to be settled there by the configuration of the sugar rather than by the registry.
The same datum is used here and the limitation is inherited unamended (Remark 9.27). But the use is positive rather than negative, and the two together say something neither says alone. A marker cannot carry a determinant; it can carry a letter. What Theorem 9.23 exhibits is a correspondence, established by an identity in $\mathbb{Z}/2$, between the sequence and the pattern of markers in the surface — exactly the kind of statement the registry is built to support, and exactly not the kind the residue account found unavailable.
The finding is entered here because it belongs to the coordination ledger rather than to either paper's own argument: the datum whose insufficiency is recorded in one place is sufficient for a different question in another, and a reader who took the recorded limitation for a general one would be misled.

Remark 13.5 (A coordination question: one generator or two)**.** [A] The excision that carves a retained subgraph and the scission that carves a chain are both cut sets on X, and Remark 5.22 shows that they act at a common edge. Whether they are one generator under different cut sets, or two, is settled by neither paper.
The question is not idle. If they are one, the architecture makes residues and membrane tails by a single operation applied to different substrates, and the common edge is a consequence rather than a coincidence. If they are two, the two branches are related only by sharing a graph, and the coincidence at C5–C6 is what it appears to be. Nothing in either paper decides it, and nothing in this one depends on the answer: both readings leave Section 5 as it stands.
It is put to the reachability development, where the generators are defined, and is Target 14.12.

Ruling 13.6 (Disposition against the patents)**.** [C] *Consistent; imported and unamended. Taken from the patent record: the two tethers with their extensions and caps (Notation 2.3); the sense in which each lays its tether along the substituted positions (Definition 4.7), which carries Theorem 9.23; the single and doubly bridged forms of the unrecruited dimer (Proposition 4.9); and the encoding scheme under which a tethered nucleic acid arises at all. Nothing of the record is*

amended here, and no result of this paper is asserted of any structure the record does not exhibit.

Remark 13.7 (What the corpus may now cite)**.** [A] Three entries, of which two belong to other papers' ledgers rather than to this paper's results.
That the edge C5–C6 is the reactive locus of both branches of the arc, which bears on the residue account's treatment of its own excision and on the reachability development's ordering of generators.
That the orientation marker, recorded as unable to settle a determinant, settles a sequence-to-surface correspondence (Remark 13.4). This belongs in the coordination ledger and should be stated when the registry's capacity is next taken up.
And that the unrecruited remainder of a pool has a use. The corpus has treated units not consumed in an encoding as remainder; Sections 5 and 6 give them a product and Section 10 gives the ratio at which they are required. Whether a pool of that ratio is available is a question for the assembly literature and is Target 14.9.

14 Targets, and conclusion

14.1 Targets, aggregated

The targets are given in the order in which settling them would do the most for the account, which is not the order in which they arise. The first three are premises on which whole sections stand; the remainder fix figures or close questions the account can carry open.

Target 14.1 (The folded arm)**.** Determine whether the capped arm folds into one leaflet or extends across the core. It is H7. Fully extended the unit measures 30 to 33 Å against a hydrophobic core of 27, so the arm must lose 2.8 to 5.5 Å of its eleven; a freely jointed estimate gives 3.8, an unforced loss of 7.6, which is ample but is an estimate. Sections 8 and 9.2 have a subject only if it folds, and this should be settled before anything else in this list.

Target 14.2 (The regime)**.** Decide dispersal against aggregation for units of the footprint of Corollary 7.8 in a surface of the composition of Section 6. It is H2, and it is placed second because the prior runs against it. The same π-stacking this paper assumes away is what holds the corpus's cluster together; the units are placed here in the disposition in which aromatic faces contact one another laterally, a face of 12.5×7.0 Å standing with the normal in its plane; and aggregation would not weaken Sections 8 and 9 but replace their subject. Dispersal is the surprising branch and carries the burden.

Target 14.3 (Face freedom)**.** Determine whether the nucleoside arm permits a unit to present either face while delivering its nucleoside to the interface. It is H8, and it is the premise on which the second of the source's two bits has a carrier. By Theorem 9.24 it decides whether the surface holds the whole base-four word at two bits per anchor or half of it at one, losing the polarity of every pair. The question is conformational and is finite once the arm's rotamer states are enumerated — the same enumeration Target 14.1 requires, which is a reason to take the two together.

Target 14.4 (The minority component)**.** Determine the proportion of macrocyclic to singly bridged dimers, and whether the macrocycle's product is accommodated as a spanning species in a bilayer of the route-A lipid. It spans about fifteen Å against the twenty-seven of that bilayer, so it is short for the office and would span a thinned region rather than the membrane at rest. The proportion is not supplied by the record and the accommodation is not settled here.

Target 14.5 (Partial anchoring)**.** Determine whether an anchor can fail to form on the compartment opposite to the strand, and what a partially anchored strand does to the anchor count. This is the live form of H3, the no-threading premise: under Proposition 8.6 the strand does not thread the core, so what fails instead is the anchoring, and unlike threading it leaves a trace in a quantity the paper computes.

Target 14.6 (The fate of the ether, and the geometry it leaves)**.** Decide first between retention and elimination at the C6 ether: under retention the tail carries a mid-chain ether at carbon ten, under elimination a double bond there. Then, given elimination, determine whether the double bond is *cis* or *trans*. The position is fixed by the cut set and the geometry is not. A *trans* product is a gel-phase membrane and would make Hypothesis 7.16 and the lateral diffusion of Proposition 3.1(iv) both false, leaving an account of a different object.

Target 14.7 (The cap, and the acceptance windows)**.** Determine the perturbation of chain order produced by the branched isopropyl cap against the linear ethyl cap at the same backbone depth, and compute $W_{\ell_{\mathrm{A}}}$ and $W_{\ell_{\mathrm{C}}}$ from the tether geometry. Together they fix the capacity of Section 9.3. The section is the weaker of the two channels and

is not load-bearing, so these may be carried open.

Target 14.8 (The head-group area)**.** Compute the head-group area of the lipid of Corollary 5.21 rather than taking it at a literature value for its class. With the bending tolerance it constitutes H5, and it enters Corollary 10.6 linearly and is one of the two stipulated parameters there, the other being the bending tolerance E^{*}.

Target 14.9 (The ratio)**.** Determine whether a pool of order 10^{2} unrecruited vessels per encoded vessel is attainable in any assembly the corpus describes. What is asked is a ratio and not a count, Theorem 10.5 having removed the dependence on strand length.

Target 14.10 (The head group)**.** Establish, as a matter of fact rather than of admissibility, the source of the head-group nitrogen and of the four carbons a phosphatidylcholine requires beyond the dimer's budget. A positive answer discharges H1 and makes the phosphatidyl reading unconditional; a negative one leaves the dialkyl phosphate of Theorem 6.4, which is lamellar and suffices for every section below it.

Target 14.11 (Signalling and modulation across the tether)**.** Determine whether a perturbation of the membrane — local order, curvature, the packing about a cap — propagates along the tether to the nucleic acid, and whether the reverse path carries. This is the question the injection of Theorem 9.23 makes worth asking rather than answers: the injection is the condition without which no decoding could occur, and the tethering complex is the covalent structure along which a decoding would run. Signalling and modulation between an enclosure and the sequence it encloses are proposed here as a subject of future study and are not addressed in this paper.

Target 14.12 (One generator or two)**.** Decide whether the excision of the residue account and the scission of this paper are one generator under different cut sets. Remark 13.5 states what turns on it, which is an interpretation of the common edge and not any statement of Section 5.

14.2 Conclusion

Proposition 14.13 (What is established)**.** [A] *Subject to the register of Appendix A, and distinguished by kind:*

(i) The cut set carrying an unrecruited dimer to an amphiphile is forced up to one edge. The skeleton has cyclomatic number four and the corpus's three interior connectors are three of them, so one cycle edge among eighteen remains free; four of the eighteen are attachment-admissible and reach four topologies (Lemma 5.3, Theorem 5.10).

(ii) Of the four, one places its tails in the lamellar range. The selection is by tail length and not by topology, the macrocyclic dimer reaching the same diacyl topology at a higher cut count and shorter tails (Corollary 5.16, Remark 5.17).

(iii) Eliminating rather than reducing the ether at C6 *fixes the retained unsaturation at* Δ9*, that position standing at carbon ten of eighteen under both admissible cut sets, and the product is a di-O-(octadec-9-enyl) phosphate of formula* $\mathrm{C_{40}H_{79}O_{6}P}$ *(Theorem 5.20, Corollary 5.21). Its tail length, unsaturation position, linker size and linkage type were each fixed by the enumeration before any comparand was consulted.*

(iv) Carbon is the only element the dimer constrains, and the informative quantity is its partition and not its total. Four in the linker and thirty-six in two tails is a dialkyl phosphate diester and is lamellar; a phosphatidylcholine of the same total spends eight on a head the budget cannot supply (Convention 6.1, Theorem 6.4).

(v) The tethered unit and the lipid are the same skeleton in two states, cut and uncut, so the surface is made of the unit's own material (Convention 4.13, Remark 7.2). Its orientation in a leaflet is a tilt range rather than a direction, over which it presents a footprint of 0.39 *to* 0.43 $\mathrm{nm^{2}}$ *and a depth of fifty-two to seventy-two per cent of a leaflet (Proposition 7.6, Corollary 7.8).*

(vi) Encapsulation of an anchored strand is constancy of a $\mathbb{Z}/2$*-valued map on its anchor set, the number of core crossings being the number of sign changes (Theorem 8.3). The condition is not metric (Corollary 8.4). Since a crossing carries a charged backbone through an acyl core, the constant case is the only one with a route, and encapsulation reduces to one bit fixed at closure (Proposition 8.6, Corollary 8.8).*

(vii) The tethered unit carries the encoding rather than a reference to it: its alignment to the partner it templated and its orientation in the cluster's frame are two binary data indexing base four, and it retains them (Definition 4.7, Remark 4.8). The source is two bits per anchor (Lemma 9.12), of which the pair type is written into the molecule as a tether and a cap and is carried unconditionally (Lemma 9.13).

(viii) A closed surface supplies the frame the remaining bit requires. Its normal is globally defined, so the face a unit presents away from the mid-plane is one question at every anchor, and the anchors encode collectively rather than severally. No other datum of a fluid surface serves (Proposition 9.20).

(ix) The capacity of the passage is two bits per anchor or one, according to whether the flexible arm permits either face to be presented. Under the first the map from sequence to surface state is a bijection and the base-four word transfers entire with no kernel; under the second the fibres have size 2^m and exactly the polarity of every pair is lost (Theorem 9.23, Theorem 9.24).

(x) Closure requires an unrecruited pool of order 10^2 vessels per encoded vessel, and the requirement does not grow with the sequence enclosed, R^2 being proportional to n in both confinement models (Theorem 10.5, Corollary 10.6). Because the strand is anchored rather than free the operative condition is a curvature and not a volume, which lowers the requirement about sevenfold (Remark 10.4).

Remark 14.14 (What is not established, restated)**.** [A] Four things, stated here because Proposition 14.13 reads as a list of accomplishments and a list invites over-reading.

No cell is produced. A closed surface containing a strand is not a cell, and nothing here bears on metabolism, division, transport or replication.

No closed system is exhibited. The head group of the phosphatidyl reading, the thirty-two reducing equivalents of the scission, and the setting that supplies a pool of order 10^2 are all inputs, and the paper offers a ledger of them rather than a dispensation from them.

Nothing reads the encoding. What is established is that the surface holds it. Scholium 9.30 is at length about the difference, because the distance between a configuration and a code is the whole of what remains between this paper and anything a reader will want it to mean.

And no resemblance is used as an argument. The footprint of the tethered unit brackets that of a sterol; the tail of the lipid carries its unsaturation where a membrane lipid ordinarily carries it; the total carbon of the dimer agrees with a common phosphatidylcholine. All three are recorded and none is used (Remark 7.9, Remark C.4, Remark 6.8).

Scholium 14.15 (What would overturn the paper)**.** Four findings would do it, of different weights, and the weights are as instructive as the findings.

An extended rather than folded capped arm would remove the subject. The unit would span the bilayer, the leaflet map would not be a function on anchors, and Sections 8 and 9 would concern an object that does not exist. What would remain is the scission, the ledger and the closure arithmetic, which are sound and which are about a membrane rather than about an encoding.

Aggregation rather than dispersal would replace the surface with a domain, and with it the setting in which every statement about an anchor is made.

A face slaved to the tether type would halve the capacity, leaving the pair types in the surface and losing the polarities. This is the branch the paper does not take and cannot presently exclude, and it is a loss of exactly half a result rather than of a result.

And a derivation, from the architecture alone, that the templating orientations are what Definition 4.7 says they are would refute the paper in the other direction — by establishing as a theorem what is here imported as the encoding. It is named because such a derivation might be taken for a confirmation, whereas it would in fact correct this paper's account of what it has assumed.

Scholium 14.16 (The shape of the account)**.** It is worth setting out once what carries the paper, because the premises have moved several times in the drafting and the final distribution is not the one a reader would predict.

The membrane is carried by arithmetic. That an unrecruited dimer yields a lamellar amphiphile, that its tails are eighteen carbons with unsaturation at $\Delta 9$, that its carbon partitions as four and thirty-six — these are enumerations over a graph and counts over a record, and they stand whatever becomes of any hypothesis in Appendix A.

The enclosure is carried by a parity argument and an energetic one: a $\mathbb{Z}/2$-valued map must be constant, and it is constant because the alternative carries a charged backbone through an acyl core.

The encoding is carried by a frame. That the anchors hold the sequence collectively rather than severally is true because a closed surface has a normal and for no other reason, and the capacity that rides on it is two bits per anchor or one according to a premise about the flexibility of nine backbone atoms.

Three arguments of three kinds, and the conformational content of all of them is confined to four premises. That is a smaller surface of attack than the subject usually admits, and it is also a smaller cushion: the four premises cannot be checked by inspection, and three of them are stated here without a calculation behind them.

A Hypothesis register

	premise	**what rests on it**	**what survives its failure**
H1	The head-group carbons and nitrogen are supplied from outside the dimer (Sup. 6.7).	The phosphatidylcholine reading, and nothing else.	The dialkyl phosphate reading of Thm. 6.4, which is lamellar as it stands; every statement of Sections 7 to 10, by Cor. 6.6.
H2	Tethered units disperse rather than aggregate (Hyp. 7.16).	Sections 8 and 9 entire, which are stated of units in a leaflet and not at a domain boundary.	The scission classification and the ledger, which are about cut sets and counts; the geometry of Sec. 7, which is about one unit.
H3	No anchoring forms with a sign change of λ (Hyp. 8.7), the crossing carrying a charged backbone through the acyl core.	Cor. 8.8, and with it encapsulation.	The condition itself, which is Thm. 8.3; encapsulation returns to $m-1$ bits and the strand may be transmembrane.
H4	Helical registry and the acceptance windows of the metric channel (Thm. 9.33).	Section 9.3 only.	Everything else, the orientation channel of Sec. 9.2 being independent of it; the strand partition, which is finite.
H5	The closure geometry: head area a, persistence length L_p, rise h, and the bending tolerance E^*.	The value of ν at Cor. 10.6, not its constancy.	Thm. 10.5 entire, which turns on $R^2 \propto n$ and not on any parameter value; the requirement on the pool becomes unquantified rather than false.
H8	The nucleoside arm permits either face to be presented (Hyp. 9.22). Assumed jointly with H7, which may compete with it for the same conformational freedom (Rem. 7.12).	Thm. 9.23: the second bit of the source, and with it half the channel.	The identity of α with ω, which is chemical; the surface holds one bit per anchor instead of two, losing the polarity of every pair (Thm. 9.24(ii)).
H7	The capped arm folds, so the unit lies within one leaflet (Hyp. 7.11).	Cor. 7.13, and through it Sections 8 and 9 entire — the leaflet map is not defined without it.	Sections 5 and 6 entire, the geometry of Sec. 7, and the closure arithmetic of Sec. 10. The unit spans the bilayer and the anchoring of this paper does not exist.
H6	The dimer and tether record is the corpus's and the patents'.	The ledger of Thm. 6.4 and the audit value of blocks V0 to V5.	The architectural statements, which are about cut sets on a graph and not about which record they run over.

Remark A.1 (The dependency, in one sentence)**.** [A] H6 carries the record and H2 carries the surface; H1 carries a head group and not a bilayer; H3 carries the enclosure and not the condition on it; H4 carries the capacity and not the partition; H5 carries a number and not a statement. A reader who denies H2 has no account of Sections 8 to 10 and keeps Sections 5 and 6 entire.

B Verification

Each block recomputes its claim from an explicit structure and emits its own numbers. Nothing quantitative in the body of this paper is asserted; every such statement is transcribed from a block below. Block V0 is the exception: it emits the record the other blocks run on.

V0 [COMPUTED] **The dimer and tether record**

The vessel graph topology and locant registry; the two bridge topologies of Proposition 4.9; both tethers of Notation 2.3 written atom by atom with

their lengths; the head-group inventory. This is the record blocks V1 to V7 run on, and a reader may check it against the corpus's block R9 and the figures of the two patents.

```
VESSEL GRAPH TOPOLOGY
  18-cycle: 1-2-3-4-4a-4b-5-6-6a-7-8-9-10-10a-10b-11-12-12a-1
  Chords:   C4a-C12a,  C4b-C10b,  C6a-C10a
  Substituted vertices: C6, C12
  Cycle separation C6 to C12: 9 edges of 18, which is half

BRIDGE TOPOLOGIES
  single : C12(X_n) -O-CH2CH2-O-P(=O)(O)-O-CH2CH2-O- C12(X_{n+1})
           C6 free on both units
  double : as above, and C6(X_n) ... C6(X_{n+1})      [macrocycle]

TETHERS
  T_A : C2(adenosine) -OCCOPOCCO- C6(chrysene)
        backbone atoms = 9   length l_A = 10 bonds
  T_C : C5(cytosine) -CNCOCCOPOCCO- C6(chrysene)
        backbone atoms = 12   length l_C = 13 bonds
  l_C - l_A = 3 atoms  (~3.8 A fully extended)
  the extension is the three-atom C-N-C prefix of T_C and nothing else

HEAD-GROUP INVENTORY, route A
  linker carbons per bridge : 4
  phosphorus                : 1 per bridge
  nitrogen                  : 0
  framework carbons per unit: 18   (fixed; no generator adds one)
```

V1 [COMPUTED] One cycle edge severed

Enumerate the cut sets severing the three chords and one cycle edge; emit the resulting path, its length, its endpoints, and whether each substituted vertex is terminal. Emit the count of cut sets terminal at each.

```
18-cycle: 1-2-3-4-4a-4b-5-6-6a-7-8-9-10-10a-10b-11-12-12a-(1)
chords severed in every row: C4a-C12a, C4b-C10b, C6a-C10a

  edge cut        path length   endpoints        C6 term   C12 term
  ------------------------------------------------------------------
    1-2              18            2 ..  1         no        no
    2-3              18            3 ..  2         no        no
    3-4              18            4 ..  3         no        no
    4-4a             18           4a ..  4         no        no
   4a-4b             18           4b .. 4a         no        no
   4b-5              18            5 .. 4b         no        no
    5-6              18            6 ..  5        yes        no
    6-6a             18           6a ..  6        yes        no
   6a-7              18            7 .. 6a         no        no
    7-8              18            8 ..  7         no        no
    8-9              18            9 ..  8         no        no
    9-10             18           10 ..  9         no        no
   10-10a            18          10a .. 10         no        no
  10a-10b            18          10b .. 10a        no        no
  10b-11             18           11 .. 10b        no        no
   11-12             18           12 .. 11         no       yes
   12-12a            18          12a .. 12         no       yes
  12a-1              18            1 .. 12a        no        no
  ------------------------------------------------------------------
  rows: 18;  path length 18 in every row (Hamiltonian)
  cut sets terminal at C6 : 2
  cut sets terminal at C12: 2
  cut sets terminal at both: 0   (C6 and C12 are not cycle-adjacent)
```

V2 [COMPUTED] Two cycle edges severed

Sever two cycle edges; emit the pair of chain lengths and, for each chain, which substituted vertices it contains and whether they are terminal. Emit the counts by class and print the cut sets of each admissible class in full.

```
  total two-edge cut sets                        : 153
  C6 and C12 in different chains                 :  81
  ... and both terminal in their own chain       :   2
  C6 and C12 in the same chain                   :  72
  ... and both terminal (bola chain + free chain)  :   2

  SEPARATED AND TERMINAL  (two attached chains, one per substituted vertex)
  edges cut               chains        chain A         chain B
  ------------------------------------------------------------------
```

```
  5-6    & 11-12      ( 9, 9)     6(t)            12(t)
  6-6a   & 12-12a     ( 9, 9)     12(t)           6(t)

  SAME CHAIN, BOTH TERMINAL  (one bola chain, one unattached chain)
  edges cut               chains        chain A         chain B
  ------------------------------------------------------------------
  5-6    & 12-12a     (10, 8)     6(t)+12(t)      free
  6-6a   & 11-12      ( 8,10)     free            6(t)+12(t)

  (t) terminal in its chain   (i) interior   free = no substituted vertex

  The last class leaves an unattached chain of eight and is excluded by
  Definition 5.2; it is printed because its exclusion is a finding and
  not a convention.
```

V2b [COMPUTED] Products of the doubly bridged dimer

The substrate is the macrocyclic unrecruited dimer: both substituted positions bridged, neither carrying a free ether. Emit the product of each route, the ring and tail counts, the separation of the two phosphorus centres, and the hydrophobic thickness the macrocycle can span.

```
ROUTE C   one cycle cut per unit, incident to C12
  chain per unit : 18 carbons, C12 terminal, C6 at position 10
  C12..C6 segment: 10 carbons;  beyond C6: 8 carbons (pendant tail)
  MACROCYCLE : 2 x 10 framework + 8 bridge = 28 ring carbons
               2 pendant tails of C8;  two P, diametrically placed
  carbons between the two P along one arc : 2 + 10 + 2 = 14
  total carbon: 2 x 18 + 8 = 44
  CLASS: macrocyclic bolaamphiphile -> MONOLAYER membrane, not a bilayer

ROUTE D   two cycle cuts per unit, separating C6 from C12
  cut sets {C5-C6, C11-C12} and {C6-C6a, C12-C12a} -- the only two (block V2)
  two diacyl lipids, each 2 x C9 tails + 4 C linker = C22;  total 44
  CLASS: diacyl at tails of nine -- the micelle-forming range

THE ETHER
  Both substituted positions are bridged, so there is NO FREE ETHER at C6.
  The elimination of block V2c has no substrate here: routes C and D give
  saturated tails, or tails whose unsaturation the ledger does not locate.
  The Delta-9 result and the di-O-(octadec-9-enyl) phosphate belong to the
  DOMINANT singly bridged substrate, on which the ether at C6 is free.

MEMBRANE THICKNESS, ROUTE C
  extended P--P span along one arc : 14 x 1.27 = 17.8 A
    fully extended   17.8 A
    lightly bowed    15.1 A
    strongly bowed   12.4 A
  COMPARANDS
    archaeal tetraether monolayer   ~25-30 A hydrophobic
    di-C18:1 bilayer                ~27 A
    route C monolayer               ~15 A
  Thinner than either comparand by a third or more.  Permeability rises
  steeply as a membrane thins; whether this one seals is not settled here.

THE TETHERED UNIT IN A ROUTE-C MEMBRANE
  hydrophobic thickness available : ~15 A as a single slab
  unit: skeleton 7.0-9.7 A + folded cap arm ~3.8 A = 10.8-13.5 A
  It fits, and fits more easily than within one leaflet of a bilayer
  (13.5 A).  A spanning species is moreover the NORM in a bolaamphiphile
  membrane, so H7 is relieved rather than tightened.
```

V1b [COMPUTED] Cyclomatic number and the forced cut count

The minimum number of edges a chain-forming cut set must sever, against the ring count of the skeleton and the three chords the corpus already severs.

```
  vertices V = 18    edges E = 21   (18 cycle + 3 chords)
  cyclomatic number  E - V + 1 = 4  = ring count of chrysene
  minimum edges to sever for an acyclic product: 4

  the corpus's own scission loci are the three interior connectors
      C10a-C6a,  C10b-C4b,  C12a-C4a
  severing all three leaves the 18-cycle; ONE further cycle edge is then
  both necessary and sufficient.  The cut set is forced up to that one
  choice, and block V1 enumerates the eighteen values it may take.
```

V2c [COMPUTED] The double bond left by the ether

For each admissible route-A cut set, the chain numbered from the head-bearing carbon, the position of C6 in it, and the double bond left by elimination in each of the two available senses.

```
route A, cut C11-C12
  chain numbered from C12 (carbon 1, bears the head ether):
    1:12  2:12a  3:1  4:2  5:3  6:4  7:4a  8:4b  9:5  10:6
    11:6a 12:7   13:8 14:9 15:10 16:10a 17:10b 18:11
  C6 is carbon 10; neighbours C5 (carbon 9) and C6a (carbon 11)
  elimination toward C5   -> C9=C10   = Delta-9
  elimination toward C6a  -> C10=C11  = Delta-10

route A, cut C12-C12a
  chain numbered from C12 (carbon 1):
    1:12  2:11  3:10b 4:10a 5:10  6:9  7:8  8:7  9:6a  10:6
    11:5  12:4b 13:4a 14:4  15:3  16:2 17:1 18:12a
  C6 is carbon 10; neighbours C6a (carbon 9) and C5 (carbon 11)
  elimination toward C6a  -> C9=C10   = Delta-9
  elimination toward C5   -> C10=C11  = Delta-10

  C6 is carbon 10 under both cut sets, so the reachable positions are
  Delta-9 and Delta-10 and no other.

  NOTE.  C5-C6 is the edge the residue account severs at sixteen of its
  nineteen rows.  The same edge is an elimination locus here.
```

V3b [COMPUTED] The reduction ledger and the product formula

Degrees of unsaturation of the skeleton, their discharge between ring opening and reduction, the reducing equivalents charged, and the resulting formula.

```
  chrysene C18H12:  degrees of unsaturation = 13   (4 rings + 9 C=C)
  ring openings charged to the cut set            : 4   (block V1b)
  C=C remaining to account for                    : 9
  retained as the Delta-9 of block V2c            : 1
  reduced                                         : 8
  reducing equivalents per tail   (2 H per C=C)   : 16 H
  per dimer, two tails                            : 32 H

  ROUTE A PRODUCT    R-O-CH2CH2-O-P(=O)(OH)-O-CH2CH2-O-R
    R = octadec-9-en-1-yl, C18H35, ether-linked at carbon 1
    carbons   : 2 x 18 + 4  = 40
    hydrogens : 2 x 35 + 8 + 1 = 79
    oxygens   : 6    (2 alkyl ether, 2 phosphoester, 1 P=O, 1 P-OH)
    formula   : C40H79O6P        (monoanion C40H78O6P-)

  COMPARANDS
    di-O-(octadec-9-enyl) phosphate  C40H79O6P   ether, Delta-9 x2  lamellar
    dioleoyl phosphatidic acid       C39H73O8P   ester, Delta-9 x2  lamellar
    DPPC                             C40H80NO8P  ester, saturated   lamellar

  READING.  The route-A product is the first line, not a neighbour of it.
  Tail length, unsaturation position, linker size and linkage type were each
  fixed by the enumeration before any comparand was consulted.
```

V3 [COMPUTED] The carbon budget and its partition

Carbon is the only element the dimer fixes (Convention 6.1). Emit, per route, the tail multiset, the linker carbons, the number of lipids and the carbon per lipid.

```
  Framework carbons per unit : 18   (fixed, no generator adds one)
  Linker carbons per bridge  :  4   (-OCH2CH2-O-P(=O)(O)-O-CH2CH2-O-)
  Oxygen, nitrogen, hydrogen : admitted elsewhere; placed, not counted

  route                          tails         linker C  lipids  C/lipid  C total
  ------------------------------------------------------------------------------
  A  single bridge, C12 terminal   [18, 18]          4       1       40      40
  B  single bridge, C6  terminal   [9, 8, 9, 8]      4       1       40      40
  C  double bridge, 1 cut/unit     [8, 8] + ring     8       1       44      44
  D  double bridge, 2 cuts/unit    [9, 9]            4       2       22      44
  ------------------------------------------------------------------------------
  Route A partition: 4 head : 36 tail.
```

V4 [COMPUTED] Partition against reference amphiphiles

Compare route A against four comparands on tail multiset, head carbon and nitrogen. Emit the deficits. The total-carbon column is printed and is given no weight, by Remark 6.8.

```
  reference                formula          tails      head C   N   phase
  ------------------------------------------------------------------------
  dioctadecyl phosphate    C36 O4 P         [18, 18]       0    0   bilayer
  didodecyl phosphate      C24 O4 P         [12, 12]       0    0   bilayer
  DPPC                     C40 H80 N O8 P   [16, 16]       8    1   bilayer
  DSPC                     C44 H88 N O8 P   [18, 18]       8    1   bilayer
  dinonanoyl PC            C26 H52 N O8 P   [ 9,  9]       8    1   micelle
  ------------------------------------------------------------------------

  ROUTE A (tails [18,18], head C 4, N 0) AGAINST EACH
  ------------------------------------------------------------------------------
  dioctadecyl phosphate   tails match            head C  4->0 (-4)  N +0
  didodecyl phosphate     tails [18,18]/[12,12]  head C  4->0 (-4)  N +0
  DPPC                    tails [18,18]/[16,16]  head C  4->8 (+4)  N +1
  DSPC                    tails match            head C  4->8 (+4)  N +1
  dinonanoyl PC           tails [18,18]/[9,9]    head C  4->8 (+4)  N +1
  ------------------------------------------------------------------------------

  READING.  Route A meets the dialkyl phosphate diester class without
  amendment, in tails and in head, and that class is lamellar.  It meets
  DSPC in tail length and DPPC in total carbon, and neither in partition:
  a phosphatidylcholine spends 8 carbons on glycerol and choline where the
  architecture spends 4 on its linker.  The phosphatidylcholine reading
  therefore costs one nitrogen, which is admitted, and four carbons, which
  are not in the budget.  That is Supposition 6.5, and Corollary 6.4 is the
  reason nothing below Section 6 depends on it.
```

V5 [COMPUTED] Arm inventory, tether lengths, cap differentiation, strand partition

Both arms of both units, counted atom by atom; the cap at each; the three data separating the two anchor letters; and the partition of the anchor set between the strands of a duplex.

```
ARM 1 -- to the nucleobase
  T_A  C2(adenosine) - O C C O P O C C O - C6
       backbone atoms between =  9    l_A = 10 bonds
  T_C  C5(cytosine)  - C N C O C C O P O C C O - C6
       backbone atoms between = 12    l_C = 13 bonds
  l_C - l_A = 3 atoms   (~3.8 A fully extended)

ARM 2 -- capped, at the second substituted position
  common backbone   C12 - O C C O P O C C O - R
  adenine unit  : R = ethyl      -CH2CH3       cap C = 2   arm C = 6   linear
  cytosine unit : R = isopropyl  -CH(CH3)CH3   cap C = 3   arm C = 7   branched
  backbone atoms C12 -> furthest carbon: 10 in both

THE THREE DATA THAT SEPARATE THE LETTERS
  ------------------------------------------------------------------
  datum                       adenine (a)        cytosine (c)
  ------------------------------------------------------------------
  tether length, arm 1        10                 13
  cap carbons, arm 2           2                  3
  cap shape, arm 2            linear             branched
  ------------------------------------------------------------------

  READING 1.  The data run in opposite senses on the two arms: the cytosine
  unit carries the LONGER arm and the SHORTER, WIDER cap, the adenine unit
  the SHORTER arm and the LONGER, NARROWER cap.  The differentiation is
  two-dimensional; the letters are not related by a uniform lengthening.

  READING 2.  Both caps are apolar, so arm 2 terminates in the acyl core and,
  by the opposite-faces proposition, arm 1 carries its nucleoside toward the
  interface.  Each unit is thereby oriented across its leaflet, which is what
  Definition 8.1 requires and what the earlier free-hydroxyl reading could
  not supply.

  READING 3, negative.  Both units are UNIVALENT: one nucleoside arm, one
  capped arm.  The unit graph of the earlier draft has no edges, its
  components are its vertices, and the component theorem is empty.
  Withdrawn; Appendix D.

STRAND PARTITION
  pair    anchored base   strand   tether   cap
  ----------------------------------------------------------
```

```
A-T     A               +        T_A      ethyl
T-A     A               -        T_A      ethyl
C-G     C               +        T_C      isopropyl
G-C     C               -        T_C      isopropyl
-----------------------------------------------------------
Exactly one strand of each pair is anchored; the partition is a function
of the sequence alone.

ANCHOR WORDS OF A TEST SEQUENCE
  + strand   5'-ATCGGATCCTAG-3'   (m = 12)
  position    1  2  3  4  5  6  7  8  9 10 11 12
  pair        A  T  C  G  G  A  T  C  C  T  A  G
  anchored    +  -  +  -  -  +  -  +  +  -  +  -
  tether      A  A  C  C  C  A  A  C  C  A  A  C
  w(+) carries positions [1, 3, 6, 8, 9, 11]
  w(-) carries positions [2, 4, 5, 7, 10, 12]
  |w(+)| + |w(-)| = 6 + 6 = 12 = m, so the partition is exact
  alpha = 001110011001   (pair type, carried chemically)
  beta  = 010110100101   (polarity, carried orientationally)
```

V6a [COMPUTED] The source: two bits per tethered unit

Tabulate the orientational datum of Definition 4.7 against the four bases and against the anchor chemistry, and separate the bit carried chemically from the bit carried orientationally.

```
Each tethered 6,12-disubstituted unit carries two binary data, fixed when it
templated its paired 3,6,9,12-tetrasubstituted unit:

  alpha  alignment to the paired tetrasubstituted unit (aligned/unaligned)
  beta   orientation of its rings in the cluster's common reference frame

  alpha  beta   base   anchored via   pair type
  ------------------------------------------------
    0     0      A      T_A            A-T
    0     1      T      T_A            A-T
    1     0      C      T_C            C-G
    1     1      G      T_C            C-G
  ------------------------------------------------

alpha is the PAIR TYPE and is carried CHEMICALLY: an adenine anchor bears
T_A with an ethyl cap, a cytosine anchor T_C with an isopropyl cap.  It is
a property of the molecule and no motion of the molecule loses it.

beta is the PAIR POLARITY -- which strand carries the anchor -- and is
carried ORIENTATIONALLY.  It is frame-relative and survives only if the
surface supplies a frame and leaves the unit free to record it in.

source entropy, sequence uniform over four bases: 2.00 bits per anchor
```

V6b [COMPUTED] The channel, and the capacity dichotomy

Enumerate the surface states available to an anchored unit, and count the distinct states reached over all base-four words of stated length in each branch of Theorem 9.24.

```
Orientational state of a unit inserted in a leaflet:
  lambda  which leaflet                                    (Z/2)
  omega   which substituted position faces the interface   (Z/2)
  sigma   which face is presented away from the mid-plane  (Z/2)

omega = alpha, the nucleoside arm being borne at one position only.
lambda is constant under encapsulation.  The free datum is sigma.

CASE (i)   FACE FREEDOM [H8]
           the flexible arm reaches the interface from either face, so
           sigma is free of omega and may take the value beta + c.
           capacity 2.00 bits per anchor    retained 100%

CASE (ii)  FACE SLAVED
           sigma = omega + lambda, so with lambda constant sigma is a
           function of alpha and beta has no carrier.
           capacity 1.00 bit per anchor     retained  50%

distinct surface states over all base-four words of length m
  m     words (4^m)   states, case (i)   states, case (ii)
  ------------------------------------------------------------
  1              4                 4                   2
  2             16                16                   4
```

```
  4             256               256                16
  8           65536             65536               256
  ------------------------------------------------------------

Case (i) is a bijection: no kernel.  Case (ii) has fibres of size 2^m, and
what is lost is exactly beta at every anchor -- which pairs are A-T and
which C-G is retained; which strand of each carries the anchor is not.
```

V6c [COMPUTED] The reference frame

Why beta has a carrier in a closed surface at all, and why no other datum of a fluid bilayer would serve.

```
beta is defined against the cluster's common reference frame, which does not
accompany the unit into the surface.  What replaces it is the bilayer normal:
a closed surface has a globally defined outward direction, so "which face is
presented away from the mid-plane" is one and the same question at every
anchor of the surface.

This is the condition under which the anchors encode COLLECTIVELY rather than
severally.  Were the available frame local, each anchor would carry a bit
referred to its own neighbourhood, no pattern over anchors would be defined,
and the sequence would be present in the surface in no sense at all.

No other datum of a fluid surface serves:
  position          diffuses laterally
  nearest neighbour exchanges
  azimuth in plane  has no globally defined reference direction
  tilt              is continuous and is a range, not a value (block V8)
  face vs normal    is globally defined and is preserved by diffusion

The normal supplies globally what the stack supplied in the cluster, and it
is the only datum of a fluid surface that does.
```

V6d [COMPUTED] Fibre sizes, and the price of the ordering

The fibres of the map from sequence to surface state, in the two branches of Theorem 9.24; and, to price Lemma 9.16, the hypothetical reading on which only the multiset of anchor states survives.

```
   m    words 4^m   (i) ordered, free   (ii) ordered, slaved   (iii) unordered
                     fibre    states      fibre     states       fibre*  states
-------------------------------------------------------------------------------
  1             4       1         4          2          2           1       4
  2            16       1        16          4          4           2      10
  4           256       1       256         16         16          24      35
  8         65536       1     65536        256        256        2520     165
 12      16777216       1  16777216       4096       4096      369600     455
-------------------------------------------------------------------------------
* largest fibre, at the most balanced composition

Under face freedom the map is a bijection: fibre size 1 at every word, no
kernel.  Under the slaved face the fibres are uniform of size 2^m and what
is lost is exactly beta at every anchor.  Were the ORDERING lost as well,
the fibres would grow super-exponentially and the surface would hold only
the base composition of the segment.

The ordering is supplied by the strand and costs no premise: a covalent
backbone does not permute its own residues.  Its value is the difference
between the second and third pairs of columns.
```

V6e [COMPUTED] Fibres of the metric channel

The fibres of Theorem 9.35 as a function of the engaged fraction, and the information each engagement level retains against the source's $2m$ bits.

```
an engaged anchor reports the pair type (1 bit);
an anchor out of phase reports nothing (0 bits).
fibre size = 4^(m-e) . 2^e        retained = e bits

  m     e    fibre size     retained (bits)   source 2m
-------------------------------------------------------
   8     0         65536           0             16
   8     2         16384           2             16
   8     4          4096           4             16
   8     6          1024           6             16
   8     8           256           8             16
-------------------------------------------------------
  12     0      16777216           0             24
```

```
  12     3       2097152           3             24
  12     6        262144           6             24
  12     9         32768           9             24
  12    12          4096          12             24
------------------------------------------------------------

At FULL engagement the metric channel still reports only m bits of the 2m
the source carries: the polarity has no metric carrier at any e.  The
acceptance windows therefore fix e and not the formula, and the channel
adds redundancy rather than capacity (Rem. on the two channels compared).
```

V7 [COMPUTED] Closure geometry and the pool ratio

Emit, at six strand lengths and in both confinement models, the required radius, the lipid count, and the unrecruited vessels per encoded vessel. Emit the closed forms.

```
h = 0.34 nm/bp    Lp = 50 nm    a = 0.65 nm^2    E* = 10 kT
lipids per vessel (route A, one lipid per dimer) = 0.5
encoded cluster taken at one vessel per base pair

MODEL 1 -- strand free in the lumen          R^2 >= Lp.L/3
MODEL 2 -- strand anchored to inner leaflet  R^2 >= Lp.L/(2E*)     <- this paper

  n (bp)    L (nm)   R1 (nm)   N1 lipids   nu1     R2 (nm)   N2 lipids   nu2
-------------------------------------------------------------------------------
     100      34.0      18.0       12528     251       9.2        3287      66
     300     102.0      41.2       65732     438      16.0        9860      66
    1000     340.0      75.3      219106     438      29.2       32866      66
    3000    1020.0     130.4      657318     438      50.5       98598      66
   10000    3400.0     238.0     2191059     438      92.2      328659      66
   30000   10200.0     412.3     6573178     438     159.7      985977      66
-------------------------------------------------------------------------------

CLOSED FORMS  (L >> Lp)
  model 1    nu = 16.pi.Lp.h / (3.a)   = 438
  model 2    nu =  8.pi.Lp.h / (a.E*)  =  66

READING.  In both models R^2 is proportional to n, so N is proportional to n
and nu is INDEPENDENT of the strand length WHEREVER THE MODEL APPLIES.  The
pool requirement does not deteriorate with the length of the sequence
enclosed; only the constant differs between the models, by a factor of
about seven.

ONE RESTRICTION, VISIBLE IN THE FIRST ROW.  Model 1 is a coil estimate and
needs contour length above the persistence length, that is n > 147 bp.  The
n = 100 row lies below that threshold, takes the short-chain branch, and
reads nu1 = 251 rather than 438.  Model 2 carries no such restriction and
is flat at every row; nu2 is the figure Corollary 10.6 rests on.
```

V7b [COMPUTED] Sensitivity, and the sign of each omission

Sweep the parameters of model 2 one at a time; then list what the model leaves out, with the direction in which each omission moves ν.

```
nu2 = 8.pi.Lp.h / (a.E*)      one parameter varied, the rest at base

  parameter        nu2
  --------------------
  base              66
  Lp = 30 nm        39
  Lp = 80 nm       105
  a  = 0.50         85
  a  = 0.80         53
  E* =  3 kT       219
  E* = 30 kT        22
  --------------------

nu spans about one order over plausible parameters, from a few tens to a few
hundreds.  The order is 10^2, not 10^3-10^4.  Lp is salt-dependent and a is
taken for the class rather than computed for this lipid (Target: head area).

WHAT IS NOT IN THE MODEL, AND WHICH WAY IT RUNS
  RAISES nu   the poly-adenosine-chrysene initialiser, occupying lumen the
              model does not charge for
  RAISES nu   electrostatic cost of confining a polyanion with counterions,
              absent from the bending term
  RAISES nu   any excess of R over its floor, entering as R^2
  LOWERS nu   the tethered units themselves, which occupy leaflet area and
```

```
              displace unrecruited lipid one for one by their footprint; the
              table does not credit this, so the figures OVERSTATE nu
```

V8 [COMPUTED] Embedding, locants, orientation sweep, and the arm budget

Construct the skeleton on an ideal hexagonal lattice; recover the locants from the chord pattern rather than assigning them; locate C6 and C12; then sweep the tilt of the bilayer normal within the molecular plane, emitting depth, footprint, the depth separation of the two substituted positions, and the length of the unit with both arms extended.

```
construction: ideal hexagonal lattice, aromatic C-C = 1.40 A, four
cata-condensed rings in the chrysene zigzag
vertices 18   edges 21   fusion bonds 3
locants RECOVERED, not assigned: the unique labelling of the perimeter
cycle whose fusion bonds are C4a-C12a, C4b-C10b, C6a-C10a

skeleton extents      long axis  9.10 A    short axis  3.64 A
plane thickness (pi contact)                         3.40 A

C6  at ( 4.90, -1.21)   ring C  (interior)
C12 at ( 1.40,  2.42)   ring B  (interior)
C6 -> C12 : separation 5.05 A
            3.50 A along the long axis, 3.64 A across it
            as a LINE, 46 deg to the long axis
            as a VECTOR, bearing 133.9 deg

THE TWO ANGLES ARE NOT INTERCHANGEABLE.  Only the bearing governs the depth
separation: dz vanishes where the normal stands perpendicular to the vector,
at phi = 43.9 deg.  A tilt near 46 deg is therefore the WORST case for the
separation and not the best -- the sweep below reads dz = 0.10 A at 45 deg
against 3.64 A at 90.  An earlier form of Proposition 7.6 took the line
angle for the vector and made 46 deg the lower end of the admissible
window; the correction is at Remark 7.7 and Appendix D.6.

NOT at opposite ends of the long axis.  Cycle antipodality is a property of
the perimeter walk, which passes through the interior rings.

ORIENTATION SWEEP.  phi = angle of the bilayer normal within the molecular
plane, measured from the long axis.  Admissible phi are those giving the two
substituted positions a depth separation, i.e. phi between the short-axis
direction (90 deg) and the C6->C12 direction (46 deg).

 phi   depth   width  footprint  footprint  dz(C6,C12)  arm budget
(deg)   (A)     (A)    (A^2)      (nm^2)       (A)          (A)
-----------------------------------------------------------------
   0    12.50    7.04    23.9      0.239       3.50        35.4
  15    12.50    7.82    26.6      0.266       2.44        35.4
  30    11.89    8.30    28.2      0.282       1.21        34.7
  45    11.42    9.70    33.0      0.330       0.10        34.3
  60    10.40   10.67    36.3      0.363       1.40        33.3
  75     8.91   11.88    40.4      0.404       2.61        31.8
  90     7.04   12.50    42.5      0.425       3.64        29.9
-----------------------------------------------------------------

ADMISSIBLE RANGE.  The criterion is NOT the bearing above but the
requirement that the unit lie within ONE LEAFLET: the skeleton depth along
the normal, plus the capped arm folded to its freely jointed extent, must
not exceed the leaflet half-thickness.
    folded arm, freely jointed   sqrt(9) x 1.27 =  3.81 A
    leaflet half-thickness                        13.5  A
    hence depth <= 9.69 A,  hence phi >= 67.7 deg
  a range of 22 deg, abutting the short-axis direction

  depth      7.0 to  9.7 A   =  52 to 72% of a 13.5 A leaflet
  footprint  0.386 to 0.425 nm^2  =  1.9 to 2.1 acyl chains
             (cholesterol ring system, for comparison, 0.38 nm^2)

ARM BUDGET
  arm 1 extended                        11.4 A
  skeleton, C6 to C12 along the normal   7.0 to  9.7 A
  arm 2 extended                        11.4 A
  TOTAL extended                        29.8 to 32.5 A
  hydrophobic core, two leaflets        27.0 A
  excess                                 2.8 to  5.5 A

Arm 2 must therefore lose 2.8 to 5.5 A of its 11.4 A extension to bring the
unit within one leaflet.  A freely jointed estimate of its end-to-end
extension is sqrt(9) x 1.27 = 3.8 A -- an unforced loss of 7.6 A, which
exceeds the 5.5 A the shallowest admissible tilt asks of it, with the
```

```
margin widest at the deepest tilt.  This is H7, and it is met across the
range with room in hand.

AGAINST THE WITHDRAWN GEOMETRY (long axis along the normal, Appendix D)
  depth was 12.50 A and the excess over the core 8.4 A; the excess is now
  2.8 to 5.5 A, and H7 is correspondingly less demanding.
```

C Molecular commentary, isolated

Remark C.1 (Status of this appendix)**.** [A] Nothing in this appendix enters a numbered statement, and no statement of this paper is weakened by its removal. It is retained because the observations are natural ones for a reader to make at the point where the unit enters the surface, and a paper that omitted them would invite a reader to supply them in a load-bearing place.

Remark C.2 (The sterol reading)**.** [E] A fused tetracyclic standing in a leaflet with a polar attachment at one end invites comparison with cholesterol, and the comparison survives one test: by Corollary 7.8 the footprint of 0.39 to 0.43 nm^2 brackets the 0.38 usually given for the sterol ring system, and the depth spans a comparable fraction of a leaflet.
It fails the others, and the failures are the ones that matter for what a sterol is known to do. Cholesterol is non-planar, so it cannot stack; largely saturated, so its surface is not a π face; chiral at eight centres, so its two sides are not equivalent; and anchored by a hydroxyl that hydrogen bonds at a definite depth, so its position along the normal is fixed rather than tilted over a range. The chrysene unit is planar, aromatic, achiral in its skeleton, and anchored by a phosphodiester at the end of a flexible arm. The ordering of chains without crystallisation for which a sterol is cited follows from exactly the properties the unit lacks.
An agreement in footprint between objects differing in four respects is a coincidence of size. It is recorded here and used nowhere.

Remark C.3 (Packing, and the direction of the perturbation)**.** [E] Three observations about what a unit of this shape would do to the chains around it, none of which enters a proof.
A rigid planar insert standing with the normal in its plane presents a flat face of 12.5×7.0 Å to its neighbours. Aromatic faces of that size in contact are the disposition in which π stacking occurs, and Remark 7.17 is the numbered form of the concern.
The unit reaches only fifty-two to seventy-two per cent of a leaflet's hydrophobic depth, so the region below it — the mid-plane region, where chain order is lowest in any bilayer — is occupied by the folded capped arm rather than by the skeleton. Whether a folded phosphodiester arm is tolerated there is the substance of H7 and is not settled by any observation in this appendix.
The branched isopropyl cap and the linear ethyl cap sit at the same backbone depth by Lemma 2.4, and a branched terminus disorders the chains about it where a linear one does not. This is the physical content of Remark 9.8 and the quantity Target 14.7 asks for.

Remark C.4 (The mid-chain feature of the lipid)**.** [E] The lipid of Corollary 5.21 carries its unsaturation at Δ9, which is where a monounsaturated membrane lipid ordinarily carries it, and the coincidence is worth noticing and not worth arguing from. Under retention rather than elimination the same carbon would bear an ether oxygen instead, and a mid-chain ether in an otherwise saturated tail is a motif that occurs in archaeal membranes, where it accompanies branching rather than unsaturation. Neither observation bears on which fate the ether takes, which is Target 14.6.

D What was withdrawn in preparing this paper

Remark D.1 (The spatial-pattern reading of the encoding)**.** [A] An earlier framing held that the sequence is written into the membrane as an arrangement of anchors. Lateral diffusion destroys any such arrangement on a timescale far below any process the account describes. What replaced it is the composition statement of Corollary 9.38, which is weaker, is isotopy-invariant, and is the part that survives.

Remark D.2 (The closed-system reading)**.** [A] An earlier framing held that the enclosure arises without exogenous material. The nitrogen ledger of Theorem 6.4 refutes it. What replaced it is Remark 6.9: no material beyond what the corpus already admits.

Remark D.3 (The bivalent reading of the anchor units)**.** [A] An earlier draft read the second substituted position of the adenine unit as carrying a second nucleoside and that of the cytosine unit as carrying a free hydroxyl. On that reading the adenine units were bivalent; they induced a

graph on the anchor set of a strand; and the leaflet map, constrained along each edge by a single parity, was determined on each connected component by one value. The degrees of freedom of λ were then governed by the number of components and not by the number of anchors, which was the draft's principal result about encapsulation.
Both units carry a capped alkyl arm at that position: ethyl at the adenine unit and isopropyl at the cytosine unit. Both are therefore univalent, the graph has no edges, its components are its vertices, and the theorem is empty. It is withdrawn entire, together with the face-concordance hypothesis it rested on and the two corollaries it carried.
Nothing replaces it in kind. What the caps supply instead is Proposition 9.6, a statement about one unit rather than about a pair, and one the free-hydroxyl reading could not have supplied at all: a polar terminus at that position would have stood at the interface, and the unit would have carried a polar arm on each face and no orientation.
The relation the withdrawn theorem was after is recovered at Theorem 9.23, from a different datum and in a stronger form. There the relations were edges of a graph built from unit valence and determined λ only up to one value per component; here they come from the sequence and determine it pointwise. The withdrawal therefore stands as a withdrawal — the construction was wrong and its premise was false — and is not to be read as a statement that the question it addressed is unanswered.

Remark D.4 (The assembly-order premise)**.** [A] An earlier form of Section 8 rested constancy of the leaflet map on a premise about the order of assembly — that the surface closes about an already anchored strand — and recorded that premise as the paper's most dangerous, on the ground that a threaded strand and an enclosed strand agree in every quantity the paper computes.
The premise is replaced by Proposition 8.6, which does not require it: a sign change carries a charged backbone through an acyl core, and the cost is prohibitive without reference to when the surface closed. The accompanying assessment was also wrong in its direction. What can fail is not that the strand threads the core but that an anchor fails to form opposite to it, and a partially anchored strand is distinguishable from a fully anchored one in the anchor count, which the paper computes. The failure mode is therefore visible where the earlier one was not, and Remark 8.9 states the correction where it is felt.

Remark D.5 (The long-axis orientation)**.** [A] An earlier form of Section 7 inferred from the cycle antipodality of C6 and C12 that the two arms leave the skeleton at opposite ends of its long axis, and concluded that the long axis stands along the bilayer normal. The skeleton was then given a depth of 12.5 Å and a footprint of 0.239 nm^2, and the unit with both arms extended a length of 35.4 Å against a core of 27.
Antipodality on the perimeter cycle is not antipodality in the plane. C6 lies on ring C and C12 on ring B, both interior, and the line joining them runs at 46° to the long axis over 5.05 Å. The long axis therefore does not stand along the normal, the orientation is a tilt range rather than a direction, and the figures are replaced by those of Corollary 7.8: depth 7.0 to 9.7 Å, footprint 0.39 to 0.43 nm^2, extended length 30 to 33 Å.
The error was found by computing the embedding with its locants recovered from the chord pattern rather than assigning them by hand, which is what block V8 now does and what the earlier block did not.

Remark D.6 (The tilt window, and the angle it was built on)**.** [A] The correction above left a second error behind it, of the same kind and in the same section, and it survived into the published form.
Having established that the orientation is a tilt range, an earlier form of Proposition 7.6 gave that range as the 44° between the short-axis direction and "the C6–C12 direction at 46°". The 46° is the angle between two *lines*, which is what Lemma 7.4 states and all it states; the C6–C12 *vector* lies at 133.9°. Block V8 had reported the line angle, computing it from the magnitudes of the two components, and the proposition read it as a direction.
The consequence is that the window's lower endpoint was placed within three degrees of the one tilt the proposition's own criterion forbids: at $\phi = 46°$ the depth separation of the two substituted positions is 0.18 Å, the least it takes anywhere, and it vanishes at 43.9°. The argument of the proposition yields no window at all — only that one excluded angle — and the proposition now says so.
What supplies the range is the requirement that the unit occupy one leaflet, which gives depth at most 9.7 Å and hence $\phi \gtrsim 68°$. That is a consequence of H7 rather than of the geometry, and Corollary 7.8 is relabelled [D] accordingly.
No figure moves. The intervals of Corollary 7.8 and the budget of Remark 7.10 were computed over that range throughout, and the rounding of two of them improves: depth to 9.7 Å and the excess to 2.8 Å. The error was in the derivation and not in the arithmetic, which is why it survived a check of every number in the paper and was found only when the tilt range and the intervals were recomputed against each other.

Remark D.7 (The face identity, and the one-bit reading it forced)**.** [A] An earlier draft of Section 9.2 derived an identity $\sigma = \omega + \lambda$ in $\mathbb{Z}/2$, from the requirement that the nucleoside arm reach the interface and the cap the core, together with the statement that the two arms of a unit depart toward opposite faces. It was presented as the section's principal result and as the revival of a theorem withdrawn earlier still.
The derivation assumed the arm rigidly assigned to the face of the substituted position bearing it. That is not available: the arm is a phosphodiester of nine backbone atoms, and Hypothesis 7.11 already requires it to fold back through more than that. An arm that folds can also present either face.

The identity is withdrawn, and with it the reading it forced. Under it the presented face was a function of the tether type, the surface could hold one bit per anchor, and the polarity of every base pair was lost at the passage — a conclusion the draft stated as though it were the architecture's and which was in fact an artefact of an over-rigid premise. What replaces it is Theorem 9.24, which gives that reading as one branch of a dichotomy and names the premise separating the branches.
The error was found by taking seriously what Definition 4.7 supplies. A source of two bits per anchor cannot be carried by a channel of one, and the mismatch was the signal that the channel had been described too narrowly rather than that the source had been described too richly.

Remark D.8 (The anchor as a label on the sequence)**.** [A] Earlier drafts throughout treated the tethered 6,12-disubstituted unit as an attachment to a nucleic acid, and the unrecruited units as a pool unrelated to the encoding beyond sharing a skeleton. The abstract, the introduction and Section 9 were written on that reading.
It is the reverse of the case. The disubstituted unit is the template on which its paired tetrasubstituted unit was transformed, it is not consumed in the transformation, and it retains the orientation that determined which base was made. The tether is a retained template contact, and the unit at its far end carries the encoding of the base at its near end as a property of its own geometry.
Every statement of this paper that treated the anchor as a label is withdrawn and rewritten. Nothing computed was wrong — the geometry, the ledger and the scission are indifferent to the correction — but the account of what passes into the surface was wrong in its subject, and Remark 4.8 now states the corrected reading before any use is made of it.
The word *unencoded* is retired with it. The dimer that becomes lipid is unrecruited, not unencoded: it is of the family that does the encoding and differs from a tethered unit only in never having been drawn into a complex. Convention 4.13 records the change of usage, which is not cosmetic — the retired word was doing argumentative work it had no right to, by suggesting that the material of the surface stands outside the encoding machinery when it is the same material.

Remark D.9 (The half bridges, and a substrate briefly mistaken)**.** [A] Two corrections to the bridge inventory were made in drafting and neither survives in the text, so both are recorded here.
A draft admitted *half bridges* — a phosphodiester arm terminated rather than reaching the partner — as a third bridge state, and enumerated seven configurations of a dimer, of which one was lamellar-competent, concluding that the pool ratio of Section 10 must be raised sevenfold. The inventory is withdrawn entire. The partial forms are defective units rather than designed ones, and the analysis is of the designed form.
A later draft took the unrecruited dimer to be doubly bridged throughout. On that reading no ether was free, the elimination of Theorem 5.20 had no substrate, the $\Delta 9$ position was unfixed, and route A was reachable only through a bridge cleavage stated as a supposition; what the architecture supplied directly was the monolayer of Corollary 5.12, and Sections 7 to 10 were rewritten against it. The record gives the singly bridged form as dominant and the macrocycle as a minority. The supposition is withdrawn as unnecessary, the $\Delta 9$ result and the named product are restored to [A] where that draft had marked them [D], and the bilayer is again what the architecture makes.
Part of the second draft survives and is retained: the macrocycle's product was computed there and stands at Corollary 5.12, no longer as the paper's membrane but as a minority species of the topology that spans and couples the leaflets of the majority one (Remark 5.14). The erroneous reading thus yielded a result the correct reading gave no occasion to seek.

Remark D.10 (The sterol argument)**.** [A] An earlier form argued the siting of the tethered unit from its resemblance to cholesterol. The resemblance is of ring count only, and the disanalogies are four. Replaced by Proposition 7.1, which argues from topology and does not need it.

E Sources, by use

Remark E.1 (Status of this appendix)**.** [A] A concordance, provided so that the provenance of each of the five imported statements may be checked without recourse to the source articles. It enters no proof.

source	used at	what is taken
patents [Sch25a, Sch25b], Figs. 6, 7, 9b	Prop. 4.1, Prop. 4.2, Prop. 4.3	The co-synthesis of the tether; the integrated synthesis of the 6,12-disubstituted and 3,6,9,12-tetrasubstituted chrysenes; and the doubly bridged complex at adjacent substituted positions, from which Cor. 4.4 reads the provenance of the cap.
patents, Figs. 15a–c	Not. 2.3, Def. 4.7, Prop. 4.6	The tethered complex: both tethers with their extensions and caps, and the orientational datum (α, β) whose pair indexes base four and which carries Thm. 9.23.

source	used at	what is taken
patents, Fig. 16b	Prop. 4.9, Sec. 5	The unrecruited dimer of two 6,12-disubstituted units in its singly bridged form, the substrate of routes A and B. The doubly bridged form is not exhibited there and routes C and D are carried conditionally (Rem. 5.11).
structure development [Sch26d]	Not. 2.2, Sec. 5	The vessel graph of eighteen-cycle, three chords, and locant registry; the interior connectors with scission recorded, with three of the four edges Lem. 5.3 requires.
coordinating paper [Sch26c]	Sec. 2, Sec. 13	The status labels, the locant ruling, and the four-level convention separating connectivity, chemical admissibility, geometric accessibility and physical realization, adopted at Prop. 3.1(vi).
residue account [Sch26b]	Prop. 9.5, Rem. 9.27, Rem. 5.22	That the two arms of a unit depart toward opposite faces, which carries Prop. 9.6 and through it Thm. 9.23; that an orientation marker records which orientation and not how two are related in space, inherited as a bound on what Sec. 9.2 claims; and the excision at C5–C6, against which Rem. 5.22 is stated.
cage development [Sch26a]	—	Not drawn on. The branch torsor, the cage condition and the stereochemical selection bear on a centre this paper does not form.
registry development [Sch26e]	—	Not drawn on directly. Rem. 13.4 bears on it and is entered in the coordination ledger rather than taken from it.

Remark E.2 (What is not used)**.** A The seeding and refinement apparatus, the assignment machinery, the capacity theorem and the parity obstruction are not drawn on, by Convention 4.16. No statement of this paper is affected by which assignment the registry supports, and no statement of it bears on the corpus's undecided dilemma between the selected assignment and the observed mapping.
Three literature sources are used for parameters and are not corpus material. Head-group areas and the lamellar criterion are taken from [Isr11]; bilayer thickness, acyl-chain cross-sections, sterol dimensions and lateral diffusion coefficients from [Gen89]; and helical repeat, rise per base pair and persistence length from [BCT00]. They enter Corollary 7.8, Corollary 10.6, Theorem 9.33 and Proposition 3.1(iv), and no other statement. Target 14.8 asks for the head-group area to be computed for this lipid rather than cited for its class.

References

[BCT00] Victor A. Bloomfield, Donald M. Crothers, and Ignacio Tinoco. *Nucleic Acids: Structures, Properties, and Functions*. University Science Books, 2000. Helical repeat, rise per base pair and persistence length, used at Section 9.3 and Section 10.

[Gen89] Robert B. Gennis. *Biomembranes: Molecular Structure and Function*. Springer, 1989. Bilayer thickness, acyl-chain cross-sections, sterol dimensions, and lateral diffusion coefficients, used at Section 7 and Proposition nonimp(iv).

[Isr11] Jacob N. Israelachvili. *Intermolecular and Surface Forces*. Academic Press, 3rd edition, 2011. Head-group areas, packing parameters and the lamellar–micellar criterion used at Section 5 and Section 10.

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