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AI-AUGMENTED PEER-REVIEW:

Kerogen as a Geometric Archive of the Chrysene Formalism: Macromolecular Aromatic Networks, Dimensional Signatures, and Metal Integration in Pre-Cambrian Shales

Compiled by the Editorial Office

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Review Scope and Objective

Prior to submission, this article underwent a Level 1 AI-Augmented review. Under Level 1, the author conducted an AI-augmented review of the manuscript, using review instructions provided by the editorial committee that restrict the AI system's task to identifying mathematical and logical flaws. Under Level 1, the AI-augmented review may also issue specific recommendations on how to correct identified flaws.

Upon submission, the editorial board evaluated the manuscript using the same review instructions provided to the author, in order to confirm the author-side findings. Human review was used to judge whether the manuscript adhered to the principles of the Chrysene Formalism, and whether it was grounded in the invariant chemistry that forms the axiomatic framework and tensorial space of the Chrysene Formalism. A more rigorous tier of AI-augmented peer review is currently in development and is being implemented for papers that will be published soon. It is anticipated that Level 1-reviewed papers will be subject to future audit, and, where warranted, updated versions of the manuscript may be issued.

Disclosure of AI Use

The author claims the use of AI in the development and writing of the manuscript.

AI-Augmented Review Procedure

This submission was evaluated under the journal's basic Level 1 AI-augmented review protocol, consisting of two independent stages:

(1) **Author-Side Draft Check.** During manuscript preparation, the author employed an AI-augmented review system to screen the draft for mathematical and logical flaws prior to submission.
Model(s) used: Gemini 3.1 Pro (Extended) [Preliminary Round]; Grok 4.6 [Final Round — internal iterative review].

(2) **Editorial Meta-Review.** Following submission, the editorial office conducted a second, independent check for mathematical and logical flaws, also using AI-augmentation, to verify consistency with the foundational formalism prior to acceptance.
Model(s) used: Gemini 3.1 Pro (Extended) [Preliminary Round]; Grok 4.6 [Final Round — confirmatory meta-review].

Review workflow: Two-stage sequential review. Stage 1 (Preliminary Round): both the author and the editorial office conducted an AI-augmented review using Gemini 3.1 Pro (Extended); the manuscript was cleared to advance to the Final Review Round. Stage 2 (Final Round): at the editorial office's request, the author conducted a series of internal iterative reviews using Grok 4.6, and the editorial office subsequently conducted a final confirmatory meta-review, also using Grok 4.6. Only the final meta-review of each stage is reproduced in this review record; the author's intermediate Grok 4.6 iterations are not individually included.

> **Scope of Review**
> AI-augmented review at this tier evaluates internal consistency, notational coherence, and alignment with previously established results in the formalism. It does not constitute independent verification of novel mathematical claims by a subject-matter expert, and it does not certify that a cross-field analogy

invoked in the manuscript (e.g. between a result native to one field and the formalism's invariants) is mathematically valid beyond the level of internal consistency and stated falsifiability. Readers evaluating a specific applied claim in this paper are encouraged to consult a domain specialist in the relevant field.

Part I: Preliminary Review Round

Editorial Board & Review Committee Summary (Preliminary)

Recommendation: Accept for Final Review

The manuscript successfully extends the Chrysene Formalism into the pre-Cambrian geological record by treating macromolecular aromatic networks in shale kerogen as a geometric archive of the abiotic-loom architecture. The decision to elevate the dimensional windows to a formal Corollary, to replace the earlier quasi-D_{4h} language with a metal-caged C_{2h} pair pathway, and to ground interstitial voids in lattice defects are all clear improvements in mathematical precision. The four numerical simulations provide useful, reproducible illustrations of the predicted length scales and loss of order.

The paper is well-structured, appropriately cautious in its empirical claims, and ready for publication after the minor points below are addressed.

Reviewer Comments & Author Responses (Preliminary, AI-Augmented)

1. Abstract Consistency

Critique: The abstract now correctly states the 0.34–0.38 nm stacking interval and the metal-caged rearrangement. However, one residual phrase still echoes the older "quasi-D_{4h}" formulation in spirit. A final tightening of the rearrangement sentence would eliminate any lingering ambiguity.

Author's Reply

The residual ambiguity in the rearrangement sentence has been removed. The abstract now states unambiguously that a metal ion is caged between a pair of C_{2h}-symmetric tetrasubstituted chrysene cores and that transient energy

input drives rearrangement into polycyclic architectures of altered symmetry while preserving carbon count and metal-coordination motif.

2. Roadmap Item 3

Critique: The Roadmap correctly points to the metal-caged C_{2h} pathway, yet the wording remains slightly more tentative than the Proposition in the main text. Aligning the two would improve internal consistency.

Author's Reply

Item 3 of the Roadmap has been rewritten so that its wording is identical in substance to the Proposition (metal-caged rearrangement). The two statements are now fully aligned.

3. Local Order Parameter

Critique: Definition and Proposition on the local stacking order parameter are clear. For the benefit of readers who will examine the simulation code, it would be helpful to state explicitly that the order parameter is computed only over pairs that remain within the 0.34–0.38 nm window after maturation, so that the reported decline is not an artefact of pairs that have left the geometrically allowed interval.

Author's Reply

A clarifying sentence has been added to the definition: the local order parameter is evaluated only on those stacked pairs whose separation remains inside the interval [0.34, 0.38] nm after the maturation step. This ensures that the reported decline reflects genuine loss of orientational coherence within the geometrically allowed window.

4. Defect-Generated Voids

Critique: The link between ring-opening defects and ångström-scale nucleation pockets is persuasive. A single sentence noting that the same voids remain compatible with the bridge-length spectrum of Corollary 1 would close the logical loop more tightly.

Author's Reply

The requested linking sentence has been inserted: "These defect-generated voids remain dimensionally compatible with the bridge-length spectrum already fixed by Corollary 1." The logical dependence is now explicit.

5. Simulation Figure Captions

Critique: All four simulation figures are valuable. Captions should uniformly cite the updated stacking interval [0.34, 0.38] nm and, where relevant, the local order parameter of Definition (local stacking order).

Author's Reply

Every figure caption has been updated to the interval [0.34, 0.38] nm. Captions for Simulation 2 now also reference the local order parameter by its formal definition.

6. Terminology

Critique: "Ghost pockets" and "defect-generated voids" are used interchangeably. Choosing one primary term (or explicitly equating them once) would remove a minor source of reader friction.

Author's Reply

"Defect-generated void" is adopted as the primary formal term. At its first occurrence the text notes that such voids correspond to the interstitial cavities previously termed "ghost pockets," after which the formal term is used consistently.

Author's Concluding Remarks (Preliminary)

Dear Members of the Editorial Board and Review Committee,

I thank the Committee for its careful and constructive reading of the manuscript. All six points have been addressed in the revised text. With these revisions, the manuscript is internally consistent and prepared for the next stage of editorial evaluation.

Editorial Remarks (Preliminary Phase)

The preliminary-round editorial meta-review of this manuscript has been completed. The manuscript was assessed as a well-structured revision advancing the empirical grounding of the *Chrysene Formalism*. The revisions requested above were executed to the committee's satisfaction. The manuscript was cleared to advance to the Final Review Round, where the thermodynamic boundaries and statistical simulation parameters were subjected to further geochemical scrutiny, described in Part II below.

Part II: Final Review Round

Editorial Board & Review Committee Summary (Final)

Recommendation: Accept with Minor Revisions (Secondary Review)

The author has successfully addressed all primary concerns from the first round of review. The alignment of terminology (standardizing "defect-generated void") and the strict mathematical bounding of the local stacking order parameter to the [0.34, 0.38] nm interval have significantly enhanced the rigor of the manuscript. The clarification regarding the C_{2h} to quasi-D_{4h} transition further solidifies the geometric arguments.

In this secondary review, the committee has identified a few remaining nuances primarily related to the geochemical and thermodynamic limits of the preservation archive, as well as the parameterization of the numerical simulations. Addressing these final points will ensure the manuscript is fully robust against classical geochemical critiques.

Reviewer 1 (AI-Augmented): Geochemistry & Thermodynamics

1. Thermal Maturation Limits and Graphitization

Critique: In Section 3.1, Proposition 4 states that under progressive maturation, local stacking order is lost while the stacking-distance measure remains inside the interval [0.34, 0.38] nm. However, at extreme thermal maturities (e.g., metagenesis or greenschist facies), kerogen undergoes extensive graphitization, which would physically collapse the interstitial voids and compress the π-stacking distance below 0.34 nm, destroying the abiotic-loom archive.

Recommendation: Explicitly define an upper thermal maturity bound (e.g., prior to extensive graphitization/metagenesis) for the preservation of this geometric archive. Acknowledge that the mathematical predictions of the Chrysene Formalism hold strictly within the catagenetic window before absolute thermodynamic graphitization dominates.

Author's Reply

I agree that a thermodynamic upper bound is necessary. Section 2.4 (Maturity and Preservation Constraints) and Proposition 4 have been updated. The text now explicitly defines an upper thermal maturity bound, noting that the geometric archive of the abiotic loom is preserved strictly within the diagenetic and catagenetic windows. I have added a formal caveat that

at extreme thermal maturities (metagenesis/greenschist facies), macroscopic graphitization thermodynamically collapses the interstitial voids and overrides the [0.34, 0.38] nm π-stacking parameter.

Reviewer 2 (AI-Augmented): Analytical Modeling & Simulations

2. Anisotropy in the Radial Distribution Function (Simulation 3)

Critique: Section 7.3 discusses the Radial Distribution Function $g(r)$ calculated from the ensemble of cluster centers, noting that the first significant peak coincides with the π-stacking distance. Shale kerogens frequently exhibit bedding-parallel anisotropy due to lithostatic pressure.

Recommendation: Briefly clarify whether the computed $g(r)$ in Simulation 3 assumes a purely isotropic bulk distribution or if it accounts for a localized anisotropic tensor. A short sentence characterizing the spatial assumptions of the Monte Carlo structural generation will suffice.

Author's Reply

The spatial assumptions of the simulation have been clarified. Section 7.3 now explicitly states that the computed $g(r)$ assumes a localized isotropic bulk distribution to isolate the intrinsic geometric invariants of the abiotic loom, prior to the macroscopic application of lithostatic pressure. I have noted that future anisotropic refinements will be required to model bedding-parallel compression in advanced shales.

3. Statistical Variance in Priority Measurements

Critique: Section 6.2 outlines priority measurements, such as using solid-state NMR for cluster-size distributions and SAXS/WAXS for stacking statistics. Because geological samples are inherently stochastic mixtures, the measured values will exhibit statistical variance.

Recommendation: Add a brief formal note indicating that the expected analytical results will manifest as a statistical distribution (e.g., Gaussian or log-normal) centered within the predicted geometric windows (5–15 Å and 0.35–0.40 nm), differentiating the idealized lattice parameters from the geochemically altered states.

Author's Reply

To properly frame the expected empirical data, a mathematical note has been added to Section 6.2. The text now clarifies that priority measurements (NMR, SAXS/WAXS) are expected to yield statistical distributions (e.g., Gaussian convolutions) whose means and standard deviations evaluate strictly within the predicted dimensional windows of 5–15 Å and 0.35–0.40 nm, successfully bridging the exact algebraic geometry of the lattice with the stochastic nature of geological preservation.

Reviewer 3 (AI-Augmented): Coordination Chemistry

4. Mechanistic Justification for Phosphorus-Metal Proximity

Critique: In Section 4.3, Prediction 2 states that spatially resolved analyses should reveal phosphorus enriched in the immediate vicinity of metal-bearing sites. While this is a compelling geometric prediction, the chemical mechanism driving this specific association within the defect-generated void is left unstated.
Recommendation: Provide a brief mechanistic justification in Section 4.1 for why phosphorus groups would strongly associate with these metal centers in the abiotic loom context (e.g., referencing Lewis acid/base interactions or the dielectric shielding of the defect-generated void optimizing phosphate coordination).

Author's Reply

This is a vital chemical distinction that has now been formalized. In Section 4.1, I have expanded the discussion on metal-phosphorus integration. The text now provides the mechanistic justification: the rigid, low-dielectric environment of the defect-generated void algebraically optimizes Lewis acid/base coordination, forcing exogenous phosphate substituents to act as hard ligands stabilizing the trapped metal cations (Ni, V, Fe) within the quasi-D_{4h} macrocyclic precursor.

Author's Concluding Remarks (Final)

I extend my continued gratitude to the Committee for its meticulous secondary review of this manuscript. The identification of these thermodynamic limits and simulation parameters ensures that the Chrysene Formalism is not merely treated as an abstract mathematical theory, but as a rigorously bounded physical framework applicable to real-world geochemical analysis.

With these secondary revisions, the manuscript fully accounts for the thermodynamic, statistical, and coordination-chemistry constraints of the pre-Cambrian geological record. I thank the committee for their exceptional diligence in refining this work. I believe the manuscript now meets the absolute standard of rigor required for publication in the *Annals of the Chrysene Formalism*.

Final Remarks from the Editorial Review Committee Chair

The editorial meta-review of this manuscript has been completed. Using the journal's AI-augmented evaluation protocol across both review stages, the editorial office assessed the submission's alignment between its stated mathematical formalism and its applied geochemical claims, and confirmed that the manuscript satisfies the journal's standard for internal consistency at this review tier. The manuscript's treatment of the thermal-maturity bound on preservation of the geometric archive, the isotropy assumptions underlying the radial distribution function simulation, the statistical framing of the priority measurement predictions, and the mechanistic justification for phosphorus-metal proximity was found to be consistent throughout following the secondary round of clarifications.

The manuscript is formally accepted for publication in the *Annals of the Chrysene Formalism*, Volume 1, Number 1.

Revision History

Version	Date	Notes
v1.0	2026-08-19	Initial publication.

Living Document Notice

As with any actively developing field, the mathematical and applied claims in this article are subject to periodic re-evaluation as the surrounding formalism matures and as the journal's AI-augmented review tooling advances. Consistent with standard scientific practice for provisional or fast-moving frameworks, this article and its review record may be re-audited by subsequent review systems, and a revised version bearing an updated review history may be issued to reflect developments in the field. Readers should consult the Revision History table above, and the journal's records, for the current version number and audit date of this article.

Editorial Disclaimer

The *Annals of the Chrysene Formalism* aims to develop the Chrysene Formalism through the application of advanced mathematics, using AI systems selected as well suited to this task. In pursuing this aim, it is possible that errors occur during the mathematical progression and analysis of the formalism, including within the review and editing process itself. However, the formalism is constructed within a multidisciplinary, horizontal framework that is grounded in a specific instantiation of molecular matter and its associated networks, an instantiation that is invariant and falsifiable. For this reason, the editorial office considers the formalism well suited to an AI-augmented approach, and anticipates that this approach will continue to be adapted as AI models and the surrounding mathematical understanding advance.