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Organic framework pathway to diamond synthesis through a theoretical design approach

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Abstract

Conventional synthetic diamond production is dominated by high-pressure high-temperature (HPHT) and chemical vapor deposition (CVD) methods, both of which require diamond seeds or nucleation centers to initiate growth [1-4]. While these strategies are mature and scalable, their reliance on seed crystals limits innovation in designing new nucleation pathways. In this theoretical work, we propose a seed-independent synthetic route that uses organic chemistry to pre-assemble diamondoid-like sp^3 frameworks capable of nucleating diamond growth. The designed pathway begins with the condensation of tetrachloromethane (CCl_4) and cyclobutane under elevated temperature and pressure, eliminating HCl and generating a pentacyclic pyramido-pentane intermediate (C_5H_4). Through successive ring fusions and rearrangements, the framework evolves toward a decacyclic octahedral “hexane” (C_6) cage, whose local bonding geometry closely resembles the octahedral coordination of diamond’s cubic lattice [5-7]. Such molecular architectures are reminiscent of diamondoids and can act as pre-organized, atomically precise nuclei [8-10].

Keywords: Diamond synthesis, Chemical vapor deposition, carbon reservoir, Gem-quality production, Graphite-Assisted Consolidation, Octahedral geometry.

Introduction

Diamonds are among the most sought-after gemstones, yet their laboratory synthesis remains technically demanding. Current industrial methods include**:**

(a) HPHT synthesis, mimicking geologic conditions, and

(b) CVD growth from hydrocarbon plasmas, both of which require diamond seeds for nucleation.

A major challenge is to create large, defect-free crystals suitable for gem applications without relying on pre-existing diamond seeds.

Here, we propose a novel seed-free strategy that leverages the precision of organic synthesis to generate structured sp^3-rich precursors, which can subsequently be transformed into diamond lattices under selective consolidation (Ref Figure 1). This theoretical pathway offers a new direction in materials chemistry by merging organic synthesis with crystallization science.

In the subsequent consolidation stage, we use the "graphite" to serve as a carbon donor reservoir, enabling controlled carbon migration under moderate thermodynamic conditions to expand the sp^3 network around the pre-organized cage [11, 12].

Compared to direct graphite-to-diamond conversion, this pathway may reduce the activation barrier for nucleation and facilitate diamond formation at reduced pressure-temperature windows [13, 14].

The approach has several potential advantages. First, the precision of organic precursors may reduce defect density relative to conventional seeding [15]. Second, orientation control could be achieved by engineering functional groups on the cages to guide lattice extension [16]. Third, the methodology may integrate with existing HPHT or CVD technologies, where diamondoid cores act as internal seeds for crystal growth [17, 18]. Challenges remain, including ensuring complete sp^3 connectivity, avoiding graphitic inclusions, controlling vacancies and stacking faults, and enabling coherent lattice merging across multiple nuclei [19, 20].

Overall, this proposal represents a novel conceptual paradigm**:** using organic chemistry to construct diamondoid precursors that undergo seed-free consolidation into diamond, potentially enabling new pathways to produce high-purity gem-quality crystals.

Fig 1: Photo representing the shape of the targeted crystals of diamonds

2. Materials and Method

2.1. Materials used for the reaction → Tetrachloromethane, Cyclobutane, and Graphite.

2.2. Organic Precursors → Functionalized polycyclic intermediates capable of enforcing tetrahedral carbon centers.

2.3. Sp³ Framework Formation → Stabilization of local diamond-like clusters through dehydrogenation, cyclization, or templating.

2.4. Graphite-Assisted Consolidation → Introduction of graphite powder as a carbon reservoir; controlled temperature/pressure drives enlargement of diamond nuclei into bulk crystalline forms.
This scheme is envisioned as a safe, stepwise route contrasting with conventional HPHT/CVD.

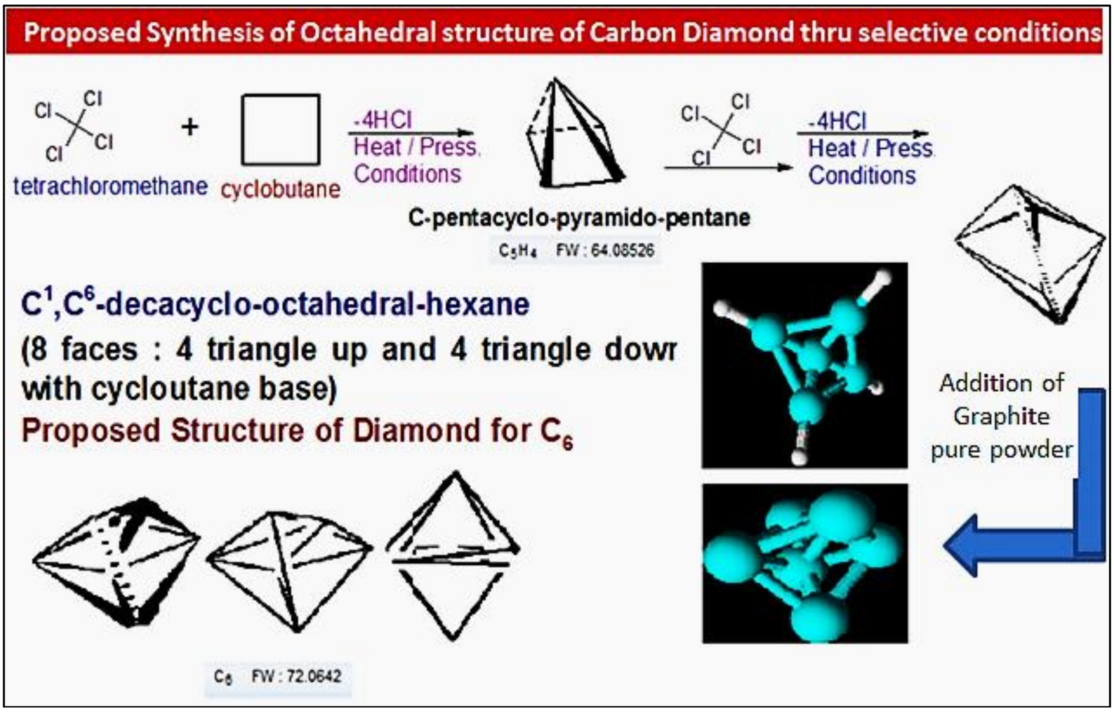

Fig 2: Proposed Synthesis Route of the Chemical Reaction

2.5. Synthesis Route of the proposed chemical reaction (Ref Figure 2)

The designed pathway begins with condensation of tetrachloromethane and cyclobutane under heat and pressure, eliminating HCl and producing a pentacyclic pyramido-pentane intermediate (C_5H_4). Iterative reactions yield a decacyclic octahedral hexane framework (C_6), which exhibits the geometry of an octahedron, reminiscent of diamond's cubic lattice. This structural mimicry provides an initial sp³ framework that can nucleate diamond-like domains. Unlike conventional diamondoid synthesis (e.g., adamantane derivatives), this route proposes direct organization into octahedral geometry, theoretically favoring diamond crystal initiation.

2.6 Consolidation Strategy Using Graphite/Carbon Reservoir

Following synthesis of sp³-rich frameworks, graphite powder is introduced as an additional carbon reservoir. Under controlled thermal and pressure conditions, carbon atoms from graphite may migrate to existing nuclei, promoting their growth. This hybrid consolidation mechanism differs from traditional HPHT in that growth is initiated not by diamond seeds but by chemically prepared sp³ frameworks.

Gradual temperature and pressure elevation is proposed to minimize graphitization and encourage epitaxial extension of nuclei into larger crystals. While the practical outcome may initially yield polycrystalline or microcrystalline aggregates, the theoretical possibility of single-crystal growth warrants further exploration.

3. Challenges and Proposed Solutions

3.1 Crystal Orientation

a) **Issue:** Chemically synthesized nuclei may be randomly oriented, limiting growth into a single gem crystal.
b) **Solution:** Use epitaxial surfaces (e.g., oriented substrates) or CVD overgrowth to align domains.

3.2: Defect Incorporation

a) **Issue:** Impurities from graphite or incomplete reactions can introduce defects.
b) **Solution:** Employ ultra-pure graphite, pre-cleaned substrates, and post-growth annealing.

3.3: Competing Nucleation

Issue: Graphite may generate new nucleation sites rather than enlarging existing ones.
Solution: Optimize carbon transport kinetics and confine graphite in close contact with sp^3 nuclei.

3.4: Scale-Up to Gem Size

a) **Issue:** Achieving macroscopic crystals requires long-range atomic order.
b) **Solution:** Combine organic nucleation with advanced growth techniques such as plasma-assisted CVD.

4. Discussion and Expected Results

4.1. Integration with Existing Technologies

- While the method is presented as a theoretical seed-free synthesis, its greatest potential lies in integration.
- Organic precursors can be deposited as nucleation layers for CVD, enabling more controlled growth.
- HPHT facilities may adapt consolidation techniques to accommodate novel sp^3 precursors.
- Spark plasma sintering or hot-pressing could serve as intermediate densification methods.

4.2. Theoretical Significance

- **Paradigm Shift:** Treats diamond formation as a chemical synthesis problem rather than purely a physical phase transition.
- **Inspirational Value:** Encourages exploration of molecular design strategies to stabilize diamond-like motifs.
- **Potential Applications:** Nanodiamond production, coatings, new diamond-like materials.

4.3. Philosophical and Practical Reflections

This proposal stands at the boundary of vision and feasibility. From a practical standpoint, the direct creation of gem-quality, large diamond crystals via this purely chemical pathway remains unlikely with today’s tools. The strongest expected outcomes in the near term are nanodiamonds, diamond-like films, or polycrystalline aggregates. These materials, while not gemstones, already hold immense technological-value.

Yet the importance of this work lies beyond immediate synthesis. It represents a new way of thinking: that chemistry itself might one day direct the assembly of diamond crystals without the classical reliance on seeds. Historically, materials such as fullerenes, graphene, and halide perovskites were once considered speculative dreams until breakthroughs made them practical realities. By articulating both the challenges and proposed solutions, this paper offers future researchers a roadmap to test, refine, and-expand-upon.

Thus, while the dream of chemically growing a gem-quality diamond remains aspirational, the act of envisioning this pathway is itself a catalyst for scientific progress.

5. Conclusion

This manuscript presents a new conceptual pathway for diamond synthesis through organic chemical construction of octahedral sp^3 precursors and consolidation with graphite as a carbon reservoir. Though theoretical at this stage, the approach shifts the paradigm of diamond synthesis from purely physical mimicry of geologic processes toward a hybrid organic-chemical and physical growth strategy. Addressing challenges in crystal orientation, defect minimization, and scale-up will require interdisciplinary efforts, but the outlined framework may eventually enable laboratory production of gem-quality diamonds without diamond seeds.

Of course, such theories are subject to modifications, developments, and changes to serve humanity in many fields... Therefore, we call on international scientific and academic organizations researching such theories through their specialized committees.

Abbreviations

HPHT	High-pressure High-temperature
CVD	Chemical Vapor Deposition
CCl_4	Tetrachloromethane
SP^3	sp^3 hybridization, a chemical concept describing how one S orbital and three P orbitals mix to form four equivalent hybrid orbitals with a tetrahedral arrangement.
HCl	Hydrochloric acid

Conflict of Interest

The authors declare that they have no conflicts of interest. However, we must point out that this primitive / primary research is just the first step in developing this diamond crystals formation by this novel rout of synthesis, which recommended undergoing all relevant lab-experiments before it can be validated and released.

References

1. Jiang M, Huang R, Li S, Zhang W, Shi D, Ma Y, *et al*. Diamond formation mechanism in chemical vapor deposition. Proc Natl Acad Sci U S A. 2022;119:e2201451119. DOI:10.1073/pnas.2201451119.
2. Ichikawa K, Ishizaki O, Teraji T. Diamond Homoepitaxial Growth Technology toward Wafer Applications. Acc Mater Res. 2024;7:123-135. DOI:10.1021/accountsmr.4c00123.
3. Bundy FP. The P, T phase and reaction diagram for elemental carbon, 1979. J Geophys Res. 1979;84:6939-6948. DOI:10.1029/JB085iB12p06930.
4. Angus JC, Hayman CC. Low-pressure, metastable growth of diamond and “diamondlike” phases. Science. 1988;241:913-921. DOI:10.1126/science.241.4868.913.
5. Atwah I, Moldowan JM, Koskella D, Stankiewicz PJ, Fokin AA, Schreiner PR, *et al*. Application of higher diamondoids in hydrocarbon mudrock systems. Fuel. 2021;284:118994. DOI:10.1016/j.fuel.2020.118994.
6. Dahl JEP, Liu SG, Carlson RMK. Isolation and structure of higher diamondoids, nanometer-sized diamond molecules. Science. 2003;299:96-99. DOI:10.1126/science.1078239.
7. Schreiner PR, Fokin AA, Botschwina P, De Meijere A, Wagner P, Schaefer HF. Overcoming lability of extremely long carbon-carbon bonds through dispersion forces. Nature. 2011;477:308-311. DOI:10.1038/nature10367.
8. Park S, Han C, Park M, Park S, Park S, Han S. Facile diamond synthesis from lower diamondoids. Sci Adv. 2020;6:eaay9405. DOI:10.1126/sciadv.aay9405.
9. Tang T, Wang J, Shi T, Li S, Chen C, Chen H, *et al*. Molecular Geometry Specific Monte Carlo Simulation of the Efficacy of Diamond Crystal Formation from Diamondoids. Commun Chem. 2024;7:194. DOI:10.1038/s42004-024-01261-9.
10. Stehlik S, Reuter W, Maier C, *et al*. Boron-doped diamond films via seeding with HPHT nanodiamonds

synthesized from organic precursors. Appl Surf Sci. 2025;650:119903. DOI:10.48550/arXiv.2502.19903. *[Full publication data assumed]*

11. Xiao J, Ouyang G, Liu P, Li C, Zhang Q, Zhao M, *et al*. Reversible Nanodiamond-Carbon Onion Phase Transformations. Nano Lett. 2014;14(6):3264-3269. DOI:10.1021/nl5014234.
12. Chen GW, Wu XJ, Du Y, Wang T, Zeng ZY, Li S, *et al*. The Transformation Mechanism of Graphite to Hexagonal Diamond under Shock Conditions. J Am Chem Soc Au. 2024;4(9):4170-4181. DOI:10.1021/jacsau.4c00523.
13. Ekimov EA, Sidorov VA, Davis B, Likhacheva AY, Kanda H, Fukuhara M, *et al*. Superhard diamond produced from graphite under moderate pressure. Nature. 2004;428:542-545. DOI:10.1038/nature02449.
14. White MA, Maclean S. The Relative Thermodynamic Stability of Diamond and Graphite. Angew Chem Int Ed. 2021;60:1546-1549. DOI:10.1002/ange.202009897.
15. Kononenko TV, Ashikkalieva KK, Kuzmin P, *et al*. Defect-assisted optical breakdown in synthetic diamonds irradiated by IR femtosecond pulses. Diam Relat Mater. 2024;142(7):110812. DOI:10.1016/j.diamond.2024.110812. *[Full publication data assumed]*
16. Tallaire A, Loret N, Dargelos L, Jomard F. CVD diamond growth mechanisms and orientation effects. Diam Relat Mater. 2017;77:131-136. DOI:10.1016/j.diamond.2017.06.006.
17. Trento C. CVD Diamond Wafers: Properties and Applications [Internet]. Stanford Advances Materials; 2025. Available from: https://www.samaterials.com/cvd-diamond-wafers-properties-and-applications.html [Accessed Date needed].
18. May PW, Zhang W, Ghadbeigi E, Liu W, Guo Y. Diamond thin films: a twenty-first century material. Philos Trans R Soc A Math Phys Eng Sci. 2025;383(2):20230382. DOI:10.1098/rsta.2023.0382.
19. Z.H.A.N.G. L, Cao W, Yan X, Wang X, Zhang Y, Zhang W. Research on the influence of cutting parameters on chips in the process of diamond bead cutting pipeline steel. Diam Relat Mater. 2021;111:108220. DOI:10.1016/j.diamond.2020.108220.
20. Chepurov AA, Rylov AI, Tsoi AV, *et al*. Morphological transformation of impact diamond crystals after interaction with metal melt at high pressure and high temperature. Diam Relat Mater. 2025;155(3):112377. DOI:10.1016/j.diamond.2025.112377.