Configuring Vertex-Integer Assignments in Carbon Fullerenes for Equal Face Sums and the Possession of the "Magic Property" for Carbon Material Engineering.

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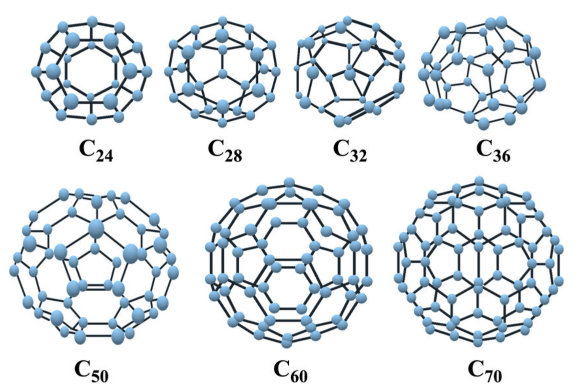
Introduction

Fullerenes are 1 of 3 Carbon allotropes with distinctive polyhedral-like geometries. They are especially useful in materials science and nanotechnology due to their unique chemical and physical properties.



Fullerene structures of C_{24}-C_{28}-C_{32}-C_{36}-C_{50}-C_{60}-C_{70}

This Project explores the existence of the "Magic Property" in fullerenes, particularly C_{60}, C_{20}, and C_{24}, where integers assigned to vertices in their pentagonal and hexagonal arrangements sum equally.Using algebraic graph theory and combinatorial mathematics, the goal of this research is to find configurations of integers on the fullerenes that could explain the chemical and physical properties especially significant in material science and engineering.

The Magic Property:

- Define a closed Polyhedron P in $\mathbb{R}^3$ with vertices $\{v_1, v_2, v_3, \ldots, v_n\}$ and define a face of the polyhedra as B_1 and all other same faces as $\{B_1, B_2, B_3, \ldots, B_n\}$.
- A polyhedron is said to have the "Magic Property" if the sum of all vertices on any B_n is equal.

Methods

This section outlines the mathematical proofs utilized to explore the "Magic Property" of fullerenes, specifically for C_{60}, C_{20}, and C_{24}, employing algebraic graph theory and combinatorial mathematics.

C_{60} Proof

Properties of C_{60}:

- 60 vertices, 12 disjoint pentagons.
- Each pentagon has 5 vertices: $12 \times 5 = 60$.
- Every vertex belongs to exactly one pentagon.

Proof:

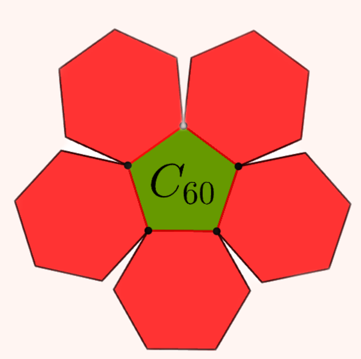
- Define $\{a_n\}$ as a sequence where $a_n = n$. Then:

$$S_{60} = \sum_{n=1}^{60} a_n = \frac{60(60+1)}{2} = 1830$$

- The sum per pentagon:

$$\frac{1830}{12} = 152.5 \notin \mathbb{Z}^+$$

- No valid integer configuration for C_{60} satisfies the property.



C_{20} Proof

Properties of C_{20}:

- 20 vertices, 12 pentagons.
- Each pentagon consists of 5 vertices: $12 \times 5 = 60$.
- Any vertex on C_{20} is shared by exactly 3 pentagons.

Proof:

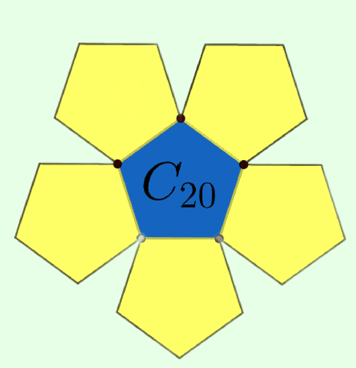
- Let $\{a_n\}$ be a sequence such that $a_n = n$. Then:

$$S_{20} = \sum_{n=1}^{20} a_n = \frac{20(20+1)}{2} = 210$$

- Since every vertex is shared by 3 pentagons, the sum per pentagon:

$$3 \times \frac{S_{20}}{12} = 52.5 \notin \mathbb{Z}^+$$

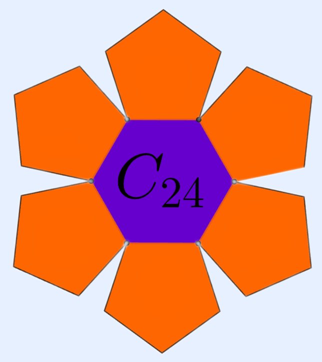
- No valid integer configuration for C_{20} satisfies the property.



C_{24} Proof

Properties of C_{24}:

- Consists of 24 vertices.
- Contains 12 pentagons.
- Contains 2 hexagons.



C_{24} Structure

Proof:

- Let S_H denote the sum of all vertices on 1 hexagonal face, and S_P denote the sum of all vertices on 1 pentagonal face.
- Let $\{a_n\}$ be a sequence such that $a_n = n$. Then, by convention:

$$S_{24} = \sum_{n=1}^{24} a_n = \frac{24(24+1)}{2} = 300$$

- By definition, every fullerene has only vertices of degree 3. Summing over all faces yields:

$$2S_H + 12S_P = 3S_{24} = 900$$

- Using the equation:

$$6S_P + S_H = 450 \quad \Longrightarrow \quad S_H = 450 - 6S_P$$

- Since S_P must be divisible by 5:

$$S_P = 5a$$

- $S_H > 0 \implies 450 - 6S_P > 0 \implies S_P < 75.$
- $S_P > 0 \implies 450 - 30a > 0 \implies a < 15.$

Table of Values for S_P and S_H:

a	$S_P = 5a$	$S_H = 450 - 30a$
1	5	420
2	10	390
3	15	360
4	20	330
5	25	300
6	30	270
7	35	240
8	40	210
9	45	180
10	50	150
11	55	120
12	60	90
13	65	60
14	70	30

Constraints:

- For S_H to be at a minimum:

$$S_H > \frac{\sum_{n=1}^{12} a_n}{2} = 39$$

- For S_H to be at a maximum:

$$S_H < \frac{\sum_{n=13}^{24} a_n}{2} = 111$$

$$\therefore \quad S_P = 60, S_H = 90 \quad \text{OR} \quad S_P = 65, S_H = 60$$

Diophantine Equations for Case 1 ($S_P = 60, S_H = 90$):

$$\begin{aligned}(v_1 + v_2 + v_3 + v_4 + v_5 + v_6) &= 60\\ (v_7 + v_8 + v_9 + v_{10} + v_{11} + v_{12}) &= 60\\ (v_3 + v_4 + v_{21} + v_{19} + v_{20}) &= 65\\ (v_4 + v_5 + v_{23} + v_{22} + v_{21}) &= 65\\ &\vdots\end{aligned}$$

Diophantine Equations for Case 2 ($S_P = 65, S_H = 60$):

$$\begin{aligned}(v_1 + v_2 + v_3 + v_4 + v_5 + v_6) &= 90\\ (v_7 + v_8 + v_9 + v_{10} + v_{11} + v_{12}) &= 90\\ (v_3 + v_4 + v_{21} + v_{19} + v_{20}) &= 60\\ (v_4 + v_5 + v_{23} + v_{22} + v_{21}) &= 60\\ &\vdots\end{aligned}$$

Results

The project explores the "Magic Property" in Carbon fullerenes by configuring integer assignments to vertices and verifying equal face sums using algebraic graph theory and combinatorial mathematics. The results show that 2 of the fullerenes, Specifically C_{60} and C_{20}, did not allow for a configuration of integers. However, C_{24}, did allow for 2 configurations of integers, as shown by the solutions to the 24-variable Diophantine equation.

1. C_{60} Proof (No Valid Configuration)
   - The total sum of integers from 1 to 60 is:

$$S_{60} = \sum_{n=1}^{60} a_n = \frac{60(60+1)}{2} = 1830$$

   - The expected sum per pentagon is:

$$\frac{1830}{12} = 152.5 \notin \mathbb{Z}^+$$

   - No integer configuration satisfies the "Magic Property."
2. C_{20} Proof (No Valid Configuration)
   - The total sum of integers from 1 to 20 is:

$$S_{20} = \sum_{n=1}^{20} a_n = \frac{20(20+1)}{2} = 210$$

   - Adjusting for shared vertices:

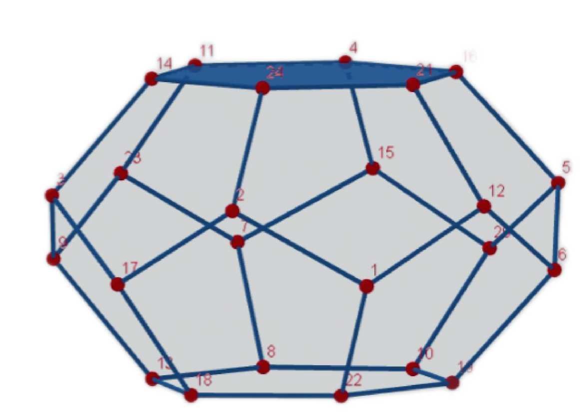
$$3 \times \frac{S_{20}}{12} = 52.5 \notin \mathbb{Z}^+$$

   - No integer configuration satisfies the "Magic Property."
3. C_{24} Proof (Two Possible Configurations)
   - Two possible configurations found:
     - $S_P = 60, S_H = 90$
     - $S_P = 65, S_H = 60$
   - The findings were validated using constraint programming and integer linear programming.
   - The computational model confirmed the impossibility of solutions for C_{60} and C_{20}.
   - The valid integer assignments for C_{24} were confirmed computationally.
   - **For Case 1, the configuration is as follows:**

$$\{v_1, v_2, v_3, \ldots, v_{24}\} = \{1, 8, 20, 17, 5, 9, 14, 4, 16, 13, 7, 6, 18, 15, 22, 10, 24, 11, 2, 23, 3, 19, 21, 12\}$$

   - **For Case 2, the configuration is as follows:**

$$\{v_1, v_2, v_3, \ldots, v_{24}\} = \{19, 10, 8, 13, 18, 22, 21, 16, 4, 11, 14, 24, 1, 12, 6, 5, 20, 15, 7, 23, 9, 3, 17, 2\}$$



Conclusion and Future Directions

Implications for Material Science:

- **Structural Stability:** The ability to assign integer values to the vertices of C_{24} for equal face sums suggests a more balanced distribution of force, which allows it to withstand significant load. This explains its usefulness in constructing composites which are especially strong and are required to be structurally solid.
- **More Reliable than C_{60} and C_{20}:** Unlike the other 2 fullerenes, which do not possess the property, C_{24} emerges more superior for material engineering because of its optimal distribution and balance of force.

Future Research Directions:

- **Computational Modeling of Other Fullerenes**: Extending these methods to C_{28}, C_{36}, and larger fullerenes to find additional structures with the "Magic Property."

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