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Research Article

Harmonic index and harmonic polynomial of some chemical graphs

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Abstract: Mathematical chemistry is a branch of mathematics that uses mathematical tools to solve chemical problems. In this paper, we calculate the harmonic index and harmonic polynomial of some chemical graphs, among graphene, star dendrimers, polyomino chains from n cycles and triangular benzene, polymolecular graphs, carbon nanotube networks, two classes of benzene-like series, nanocone, spiro chain, and polyphenylenes.

Keywords: graphene, dendrimers, spiro chain, nanocone, polymolecular graphs.

AMS Subject classification: 05C35, 05C75

1. Introduction

Mathematical chemistry is a branch of mathematics that uses mathematical tools to solve chemical problems. One of these tools is the graphical representation of chemical compounds as molecular graphs. In a molecular graph, atoms are represented as vertices, and bonds are represented as edges.
Among the various topological indices, those based on vertex degrees are particularly important and have wide applications, especially in studying quantitative structural features. These indices are used to predict the physical and chemical properties of chemical compounds, such as melting point, boiling point, flash point, molecular refraction, polar surface area, polarizability, surface tension, molar volume, and so on, without conducting laboratory experiments. One such topological index is the harmonic index [4].

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For most topological indices, a polynomial known as the topological polynomial is also defined. These polynomials provide additional information about the structure and properties of molecular graphs. The first derivative of these polynomials, evaluated at a numeric value of one, calculates the associated topological index. When calculations are performed on molecular graphs with specific structures, the ability of researchers to use graph theory or to develop a particular technique for calculations in this field is precious [6].

S. Fajtlowicz presented the harmonic index $\mathcal{H}(G)$ of a graph G in 1987, [4] which is defined as $\mathcal{H}(G) = \sum_{uv\in E(G)} \frac{2}{d_u+d_v}$. The mathematical properties of these topological indices can be found in some latest papers. Readers are encouraged to refer to [3, 9, 10] for more historical and mathematical properties of the harmonic index. Recently, Iranmanesh and Saheli presented a harmonic polynomial $\mathcal{H}(G,x)$ of graph G defined as $\mathcal{H}(G,x) = \sum_{uv\in E(G)} 2x^{d_u+d_v-1}$, where $\int_0^1 \mathcal{H}(G,x)dx = \mathcal{H}(G)$, [8]. Some mathematical results on harmonic polynomials are presented in [2]. In this article, we only consider simple connected graphs without directed and multiple edges. In the next section, the harmonic index and harmonic polynomial of some chemical graphs are computed.

2. Results and discussion

Chemical graph theory is an important branch of mathematical chemistry with many applications. In chemical graph theory, a molecular graph can be characterized by a numerical quantity called a topological index. Topological indices are classified into several major categories, among which degree-based topological indices play a prominent role in chemical graph theory. In this paper, we compute the harmonic index for some chemical graphs. So far, no chemical applications of the harmonic index have been reported. However, considering the current state of mathematical chemistry, we highlight some chemical applications of the harmonic index. The harmonic index is used in chemistry to model boiling points, molar volumes, molar refractions, heat of vaporization, surface tensions, and melting points [7].

2.1. Graphene

Graphene is a two-dimensional structure consisting of a single layer of a carbon honeycomb lattice and is one of the allotropes of carbon (see Figure 1). Graphene is a flat sheet of carbon atoms arranged in a dense honeycomb crystal lattice, with pure carbon being the primary element, which also appears in forms such as coal, fullerene, and graphite. Due to its extraordinary properties in electrical and thermal conductivity, high density, high carrier mobility, optical conductivity, and mechanical properties, graphene has become a unique material. This novel solid system is considered a very promising candidate for replacing silicon in the next generation of photonic and electronic devices. Consequently, it has attracted unprecedented attention in fundamental and applied research, represented by the symbol $G(m,n)$, [11].

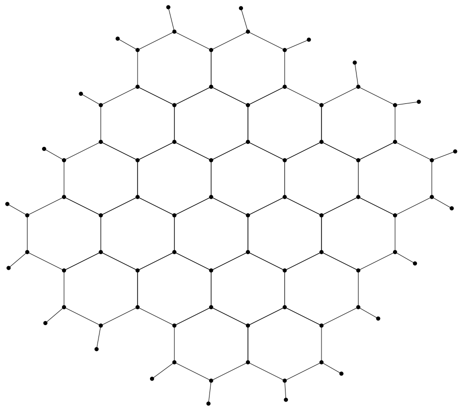

Figure 1. **2-dimensional graph of the graphene plane.**

Theorem 1. *Let $G(m,n)$ be a graphene sheet with n rows and m columns. Then*

$$\mathcal{H}(G(m,n),x) = 2(n+4)x^3 + 4(2m+n-2)x^4 + 2(3mn-2m-n-1)x^5$$

and

$$\mathcal{H}(G(m,n)) = mn + \frac{1}{30}(28m+29n+2).$$

Proof. Considering Figure 2, we have:

$$|E(G(m,n))| = \begin{cases} \left\lceil \frac{n}{2} \right\rceil (5m+1) + \left\lfloor \frac{n}{2} \right\rfloor (m+3) & \text{if} \quad n \equiv 1 \pmod 2 \\ \left\lceil \frac{n}{2} \right\rceil (5m+1) + \left\lfloor \frac{n}{2} \right\rfloor (m+3) + 2m - 1 & \text{if} \quad n \equiv 0 \pmod 2. \end{cases}$$

If $n \equiv 1 \pmod 2$, then

$$\begin{aligned} |E(G(m,n))| &= \left\lceil \frac{n}{2} \right\rceil (5m+1) + \left\lfloor \frac{n}{2} \right\rfloor (m+3) = \frac{n+1}{2}(5m+1) + \frac{n-1}{2}(m+3) \\ &= 3mn + 2(m+n) - 1. \end{aligned}$$

If $n \equiv 0 \pmod 2$, then

$$\begin{aligned} |E(G(m,n))| &= \left\lceil \frac{n}{2} \right\rceil (5m+1) + \left\lfloor \frac{n}{2} \right\rfloor (m+3) + 2m - 1 = \frac{n}{2}(5m+1) \\ &\quad + \frac{n}{2}(m+3) + 2m - 1 \\ &= 3mn + 2(m+n) - 1. \end{aligned}$$

Therefore, in each case $|E(G(m,n))| = 3mn + 2(m+n) - 1$ [5]. The partitioning of edges based on vertex degrees is shown in Table 1.

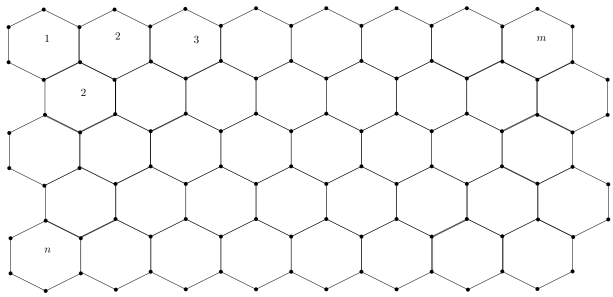

Figure 2. **2-dimensional graph of the graphene plane $G(m,n)$.**

Table 1. **The edge partition of $G(m,n)$.**

(d_u, d_v)	$(2,2)$	$(2,3)$	$(3,3)$
Number of edges	$n+4$	$4m+2n-4$	$3mn-2m-n-1$

Therefore, we obtain:

$$\mathcal{H}(G(m,n),x) = 2(n+4)x^3 + 4(2m+n-2)x^4 + 2(3mn-2m-n-1)x^5$$

and

$$\mathcal{H}(G(m,n)) = mn + \frac{1}{30}(28m+29n+2).$$

□

2.2. Star dendrimers

Dendrimers, also known as tree-like molecules, cascade molecules, or branched molecules, derive their name from the Greek word dendron, meaning tree, and mer, meaning part. Dendrimers are zero-dimensional, branched nanomolecules consisting of a central core from which multiple branching layers extend in a repetitive, tree-like manner. Each class of dendrimers is very similar in terms of size, shape, branch length, surface functional groups, and surface properties [5].
In this section, we compute the values of the harmonic index and the harmonic polynomial for three well-known infinite families of dendrimeric nanostars, namely $NS_1[n]$, $NS_2[n]$, and $NS_3[n]$, which commonly appear in pharmaceutical structures (see for example Figure 3 for $NS_1[3]$).

Theorem 2. *Let $G \in \{NS_1[n], NS_2[n], NS_3[n]\}$. Then, the harmonic index and the harmonic polynomial table are as follows:*

Table 2. **Harmonic index and harmonic polynomial of a graph G.**

G	$\mathcal{H}(G,x)$	$\mathcal{H}(G)$
$NS_1[n]$	$(18 \cdot 2^n + 8)x^3 + (36 \cdot 2^n - 24)x^4 + 6x^6$	$-\frac{68}{35} + (\frac{117}{10} \cdot 2^n)$
$NS_2[n]$	$(24 \cdot 2^n + 4)x^3 + (48 \cdot 2^n - 16)x^4 + 2x^5$	$-\frac{28}{15} + (\frac{78}{5} \cdot 2^n)$
$NS_3[n]$	$(48 \cdot 2^n - 14)x^3 + (56 \cdot 2^n - 12)x^4 + 12 \cdot 2^n x^5$	$-\frac{59}{10} + (\frac{126}{5} \cdot 2^n)$

Proof. Considering the structure of these three dendrimeric nanostars, the partitioning of edges based on vertex degrees for $NS_1[n]$, $NS_2[n]$ and $NS_3[n]$, is shown in Table 3.

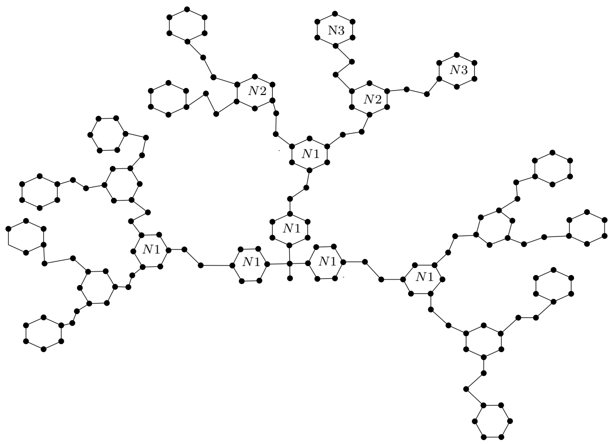

Figure 3. **Dendimeric nanostar graph $NS_1[3]$.**

Table 3. **The Edges Partition of G.**

G					
$NS_1[n]$	(d_u, d_v)	$(2,2)$	$(1,3)$	$(2,3)$	$(3,4)$
	Number of edges	$9 \cdot 2^n + 3$	1	$18 \cdot 2^n - 12$	3
$NS_2[n]$	(d_u, d_v)	$(2,2)$	$(2,3)$	$(3,3)$	-
	Number of edges	$12 \cdot 2^n + 2$	$24 \cdot 2^n - 8$	1	-
$NS_3[n]$	(d_u, d_v)	$(2,2)$	$(1,3)$	$(2,3)$	$(3,3)$
	Number of edges	$22 \cdot 2^n - 7$	$2 \cdot 2^n$	$28 \cdot 2^n - 6$	$6 \cdot 2^n$

Therefore, the result is obtained. □

In this section, we consider the important chemical graph of a star dendrimer $D_3[n]$, where n represents the number of growth stages of the star dendrimer ($n \in \mathbb{N} \cup \{0\}$). For a more detailed view of the structure of this chemical molecular graph, which appears extensively in drug structures, see Figure 4). We will compute its harmonic index and harmonic polynomial.

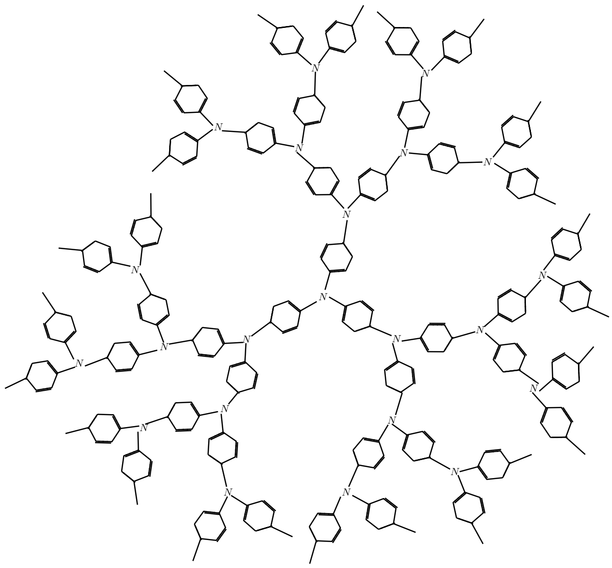

Figure 4. **Star dendrimer $D_3[n]$ two-dimensional with n growth stage.**

Theorem 3. *For the star dendrimer $D_3[n]$, we have:*

$$\mathcal{H}(D_3[n], x) = (30 \cdot 2^n - 12)x^3 + (48 \cdot 2^n - 24)x^4 + (18 \cdot 2^n - 12)x^5$$

and

$$\mathcal{H}(D_3[n]) = \frac{201}{10} \cdot 2^n - \frac{49}{5}.$$

Proof. The set of edges $D_3[n]$ can be partitioned into four parts. Therefore, we directly refer to Table 4 for its molecular structure.

Table 4. **The edge partition of $D_3[n]$.**

(d_u, d_v)	$(2,2)$	$(1,3)$	$(2,3)$	$(3,3)$
Number of edges	$6(2^{n+1} - 1)$	$3 \cdot 2^n$	$12(2^{n+1} - 1)$	$9 \cdot 2^n - 6$

Thus, according to the definition, we will have a harmonic polynomial.

$$\mathcal{H}(D_3[n], x) = (30 \cdot 2^n - 12)x^3 + (48 \cdot 2^n - 24)x^4 + (18 \cdot 2^n - 12)x^5$$

and

$$\mathcal{H}(D_3[n]) = \frac{201}{10} \cdot 2^n - \frac{49}{5}.$$

□

2.3. Polyomino chains from n cycles and triangular benzene

From a mathematical perspective, a polyomino system is a finite planar graph 2 - connected, where each internal face (cell) is enclosed by a square C_4 and formed by the union of cells connected by edges. In a polyomino chain, a square with one neighboring square is called a terminal square, and a square with two neighboring squares is called a non-terminal square. A non-terminal square has a vertex of degree 2 with a corner. A polyomino chain without corners is known as a linear chain. A polyomino chain consisting solely of corners and terminal squares is called a zigzag chain (see Figure 5). By transforming the squares into C_8 in a zigzag chain, a graph is obtained, which is referred to as a zigzag chain of 8-cycles [5] (see Figure 6).

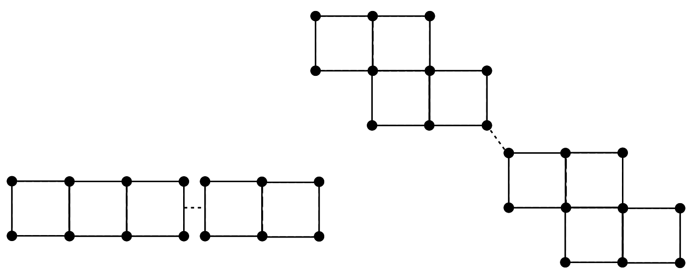

Figure 5. **An example of a linear and zigzag chain.**

Theorem 4. *Let G be a zigzag chain of 8-cycles. Then*

$$\mathcal{H}(G, x) = (24n + 8)x^3 + 16nx^4 + (16n - 6)x^5$$

and

$$\mathcal{H}(G) = 1 + \frac{178}{15}n.$$

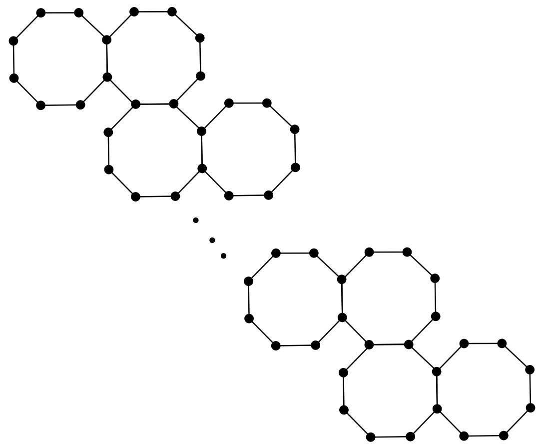

Figure 6. **Zigzag chain of 8-cycles.**

Proof. By analyzing the graph structure, the partition of edges based on vertex degrees is shown in Table 5.

Table 5. **The partition of edges in a zigzag chain of 8 -cycles.**

(d_u, d_v)	$(2,2)$	$(2,3)$	$(3,3)$
Number of edges	$12n+4$	$8n$	$8n-3$

Therefore, we obtain:

$$\mathcal{H}(G,x) = (24n+8)x^3 + 16nx^4 + (16n-6)x^5$$

and

$$\mathcal{H}(G) = 1 + \frac{178}{15}n.$$

□

The triangular benzene graph is a type of chemical graph used in chemistry and graph theory to represent the structure of certain organic molecules, particularly those that include benzene rings arranged in triangular or hexagonal configurations [1]. In this section, we obtain the harmonic index and harmonic polynomial for benzene graphs. The first class of benzene graphs we study is triangular benzene. The triangular benzene graph with n hexagon at its base is denoted by $T(n)$.

Lemma 1. *Let $T(n)$ be a triangular benzene graph with a base of n benzene. Then the number of vertices and edges is given by:*

$$|V(T(n))| = (n+2)^2 - 3 \quad and \quad |E(T(n))| = \frac{3}{2}n(n+3).$$

Proof. By counting the number of vertices at each stage and by using induction on n, we find that:

$$|V(T(n))| = (n+2)^2 - 3$$

and

$$|E(T(n))| = 3(n + \frac{n(n+1)}{2} + 1) - 3 = \frac{3}{2}(n^2 + 3n + 2) - 3 = \frac{3}{2}n(n+3).$$

□

Next, we compute the harmonic index and harmonic polynomial for the triangular benzene molecular graph $T(n)$ (see Figure 7).

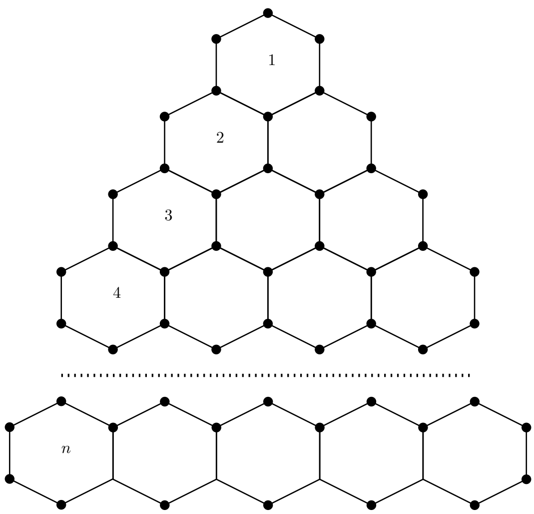

Figure 7. Triangular benzene molecular graph.

Theorem 5. *Let $T(n)$ be a triangular benzene molecular graph. Then*

$$\mathcal{H}(T(n), x) = 12x^3 + 12(n-1)x^4 + 3n(n-1)x^5$$

and

$$\mathcal{H}(T(n)) = \frac{3}{5} + \frac{19}{10}n + \frac{n^2}{2}.$$

Proof. Considering the structure of the triangular benzene molecular graph $T(n)$, there are 6 edges with endpoints of degree 2. Additionally, there are $6(n-1)$ edges with endpoints of degree 2 and 3, and there are $\frac{3n(n-1)}{2}$ edges with endpoints of degree 3. The partitioning of edges based on vertex degrees is shown in Table 6.

Table 6. **The edge partition of** $T(n)$.

(d_u, d_v)	$(2,2)$	$(2,3)$	$(3,3)$
Number of edges	6	$6(n-1)$	$\frac{3n(n-1)}{2}$

Therefore, using the definition of the harmonic polynomial, we obtain its value as follows:

$$\mathcal{H}(T(n), x) = 12x^3 + 12(n-1)x^4 + 3n(n-1)x^5 \quad \textit{and} \quad \mathcal{H}(T(n)) = \frac{3}{5} + \frac{19}{10}n + \frac{n^2}{2}.$$

□

2.4. Polymolecular graphs

Let $\{G_i\}_{i=1}^d$ be a set of finite pairwise disjoint molecular graphs with $v_i \in V(G_i)$. The bridge molecular graph $B(G_1, G_2, \cdots, G_d) = B(G_1, G_2, \cdots, G_d; v_1, v_2, \cdots, v_d)$ with respect to vertices $\{v_i\}_{i=1}^d$ is a graph obtained by taking the union of $\{G_i\}_{i=1}^d$ and adding new edges $v_i v_{i+1}$, $i = 1, 2, \cdots, d-1$, and is denoted by $B(G_1, G_2, \cdots, G_d; v_1, v_2, \cdots, v_d)$. However, if we have $v_i = v$ and $G_i = H$ for $i = 1, 2, \cdots, d$, then the symbol $G_d(H, v)$ is used [5].

In this section, we discuss polygraphs whose main components are paths, cycles, and complete molecular graphs, respectively (see Figure 8).

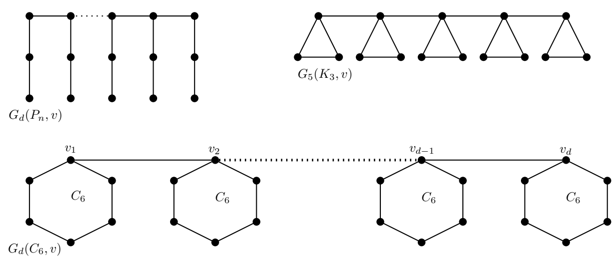

Figure 8. **Polymolecular graphs** $G_d(P_n, v)$, $G_d(C_6, v)$ **and** $G_5(K_3, v)$.

Theorem 6. *Let* $G \in \{G_d(P_n, v), G_d(C_n, v), G_d(K_n, v)\}$. *Then, the harmonic index and the harmonic polynomial table are as follows:*

Table 7. **Harmonic index and harmonic polynomial of a graph G.**

G	$\mathcal{H}(G,x)$	$\mathcal{H}(G)$
$G_d(P_n,v)$	$2dx^2+(2dn-6d+4)x^3+2dx^4+(2d-6)x^5$	$\frac{nd}{2}-\frac{d}{10}$
$G_d(C_n,v)$	$2d(n-2)x^3+8x^4+(4d-8)x^5+4x^6+(2d-6)x^7$	$\frac{37}{420}+(\frac{n}{2}-\frac{1}{12})d$
$G_d(K_n,v)$	$d(n-1)(n-2)x^{2n-3}+4(n-1)x^{2n-2}+2(d-2)(n-1)x^{2n-1}+4x^{2n}+2(d-3)x^{2n+1}$	$\frac{d(n^3+n^2-2)-2(2n^2+3n-2)}{2n(n+1)}+\frac{4(2n^2+n-2)}{4n^2-1}$

Proof. Based on the structure of the molecular graphs of the mentioned polymers, the edge partitioning according to the degrees of the vertices for $G_d(P_n,v)$, $G_d(C_n,v)$ and $G_d(K_n,v)$, are shown in Table 8.

Table 8. **The Edges Partition of G.**

G						
$G_d(P_n,v)$	(d_u,d_v)	$(1,2)$	$(2,2)$	$(2,3)$	$(3,3)$	-
	Number of edges	d	$d(n-3)+2$	d	$d-3$	-
$G_d(C_n,v)$	(d_u,d_v)	$(2,2)$	$(2,3)$	$(2,4)$	$(3,4)$	$(4,4)$
	Number of edges	$d(n-2)$	4	$2d-4$	2	$d-3$
$G_d(K_n,v)$	(d_u,d_v)	$(n-1,n-1)$	$(n,n-1)$	$(n-1,n+1)$	$(n,n+1)$	$(n+1,n+1)$
	Number of edges	$\frac{d(n-1)(n-2)}{2}$	$2(n-1)$	$(d-2)(n-1)$	2	$d-3$

Therefore, the result is obtained. □

2.5. Carbon nanotube networks

Carbon nanotubes are among the most important and widely used carbon structures that have been recently discovered. They possess unique properties and characteristics. In addition to their extremely high strength, carbon nanotubes also exhibit good flexibility and twistability. One of their applications is in composites. The most significant property of nanotubes is their electrical conductivity, which depends on the arrangement of atoms; the extent of this parameter varies accordingly [5].
In this section, we cut a rectangular piece of size $m\times n$, P_m^n by $m,n\geq 2$ from a regular hexagonal grid (honeycomb lattice) such that $m\geq 2$ hexagons are aligned along the top and bottom edges (columns) and $n\geq 2$ hexagons are aligned along the side edges (rows)(see Figure 9). The nanotube NA_m^n with $2m(n+1)$ vertices and $m(3n+2)$ edges is obtained by stacking the side edges of the rectangular piece P_m^n (Figure 9). and merging the overlapping vertices and edges. Suppose that $m,n\geq 2$ and n are even natural numbers. The tube NC_m^n of order $n(2m+1)$ and size $n(3m+\frac{1}{2})$ is obtained by stacking the top and bottom edges of P_m^n and merging the overlapping

vertices and edges [5].

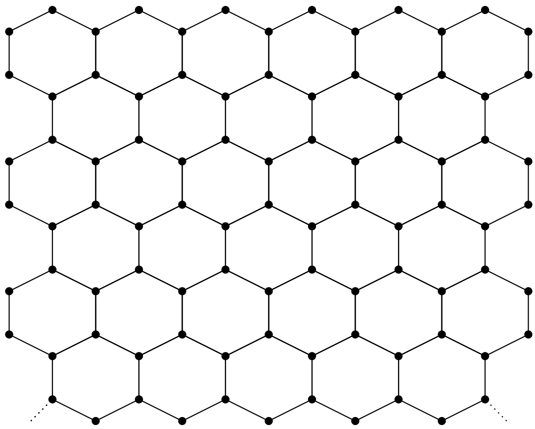

Figure 9. **Rectangular piece P_m^n Sliced from a regular hexagonal lattice.**

Theorem 7. *Let $G \in \{NA_m^n, NC_m^n\}$. Then, the harmonic index and the harmonic polynomial are in the Table 9*

Table 9. **Harmonic index and harmonic polynomial of a graph G.**

G	$\mathcal{H}(G,x)$	$\mathcal{H}(G)$
NA_m^n	$8mx^4 + 2m(3n-2)x^5$	$mn + \frac{14}{15}m$
NC_m^n	$2nx^3 + 4nx^4 + 2n(3m - \frac{5}{2})x^5$	$mn + \frac{7n}{15}$

Proof. The edge partitioning for the tubes NA_m^n and NC_m^n based on the vertex degrees is shown in Table 10.

Table 10. **The Edges Partition of G.**

G				
NA_m^n	(d_u, d_v)	$(2,3)$	$(3,3)$	-
	Number of edges	$4m$	$m(3n-2)$	-
NC_m^n	(d_u, d_v)	$(2,2)$	$(2,3)$	$(3,3)$
	Number of edges	n	$2n$	$n(3m - \frac{5}{2})$

Therefore, the result is obtained. □

2.6. Two classes of benzene-like series

In this section, our goal is to determine the harmonic index and harmonic polynomial of two classes of benzene-like series. First, we consider the circumcorone benzene-like series H_k. For $k = 1, 2, 3$, their structures are presented in Figure 10.

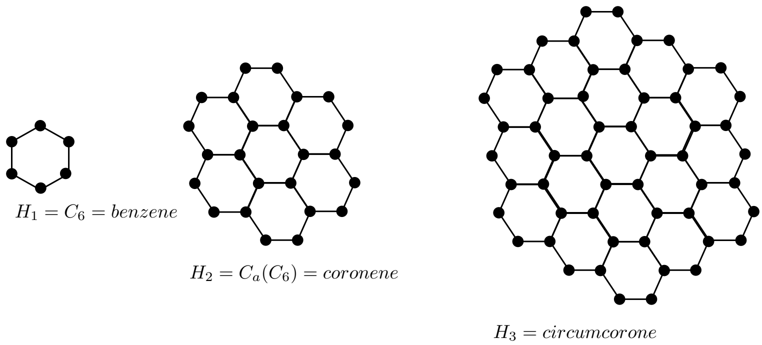

Figure 10. **The molecular graph structures of benzene, coronene, and circumcorone.**

One of the important family of molecular graphs, which consist of several copies of benzene C_6 on circumference, is the circumcoronene. For further details on this structure, we refer to Figure 11.
It is worth mentioning that coronene, also known as superbenzene, is a polycyclic aromatic hydrocarbon consisting of six benzene rings. Coronene is a yellow compound that dissolves in certain organic solvents such as benzene, toluene, and dichloromethane. The resulting solutions emit blue fluorescence under ultraviolet light [5].

Theorem 8.

$$\mathcal{H}(H_k, x) = 12x^3 + 24(k-1)x^4 + (18k^2 - 30k + 12)x^5$$

and

$$\mathcal{H}(H_k) = 3k^2 - \frac{k}{5} + \frac{1}{5}.$$

Proof. Consider the Kronenbourg benzene-like series H_k with $k \geq 1$. It is easily seen that H_k has $6k^2$ vertices and $9k^2 - 3k$ edges. Additionally, it is concluded that the partition of the edges of H_k based on the degrees of the vertices is shown in Table 11.

Table 11. **The edge partition of H_k.**

(d_u, d_v)	$(2,2)$	$(2,3)$	$(3,3)$
Number of edges	6	$12(k-1)$	$9k^2 - 5k + 6$

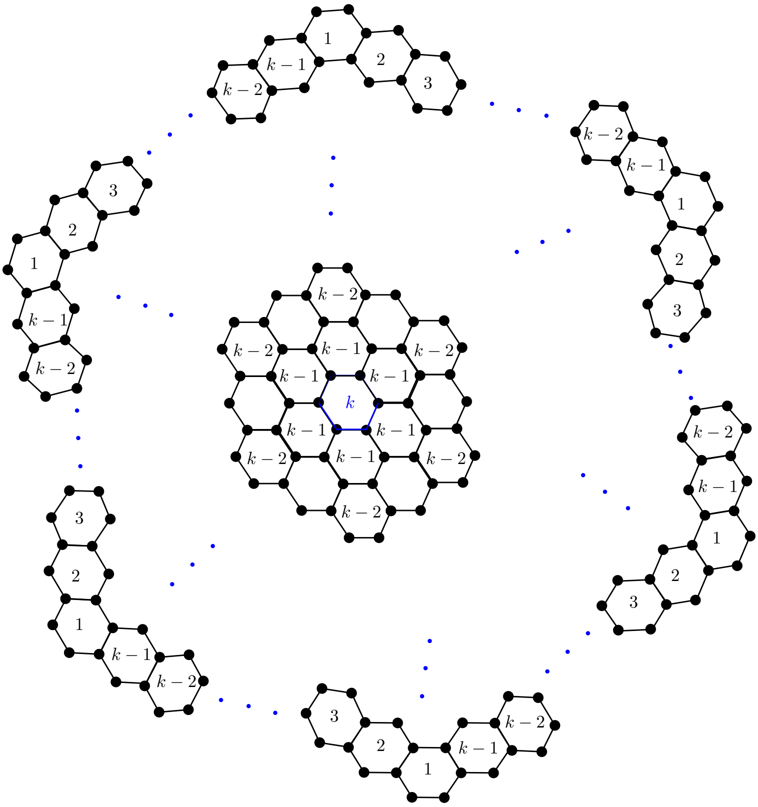

Figure 11. **The circumcoronene series of benzenoid H_k, for $k \geq 1$.**

Thus, according to the definition, we will have a harmonic polynomial.

$$\mathcal{H}(H_k, x) = 12x^3 + 24(k-1)x^4 + (18k^2 - 30k + 12)x^5$$

and

$$\mathcal{H}(H_k) = 3k^2 - \frac{k}{5} + \frac{1}{5}.$$

□

Capra transforms of a planar benzenoid series are a family of molecular graphs which are generalizations of benzene molecule C_6. In other words, we consider the base member of this family to be the planar benzene, denoted here by $C_{a_k}(C_6)$. Next, we consider the planar benzene-like series with the Capra design. Further details can be found in [5]. We will calculate the harmonic index and the polynomial $C_{a_k}(C_6)$ in the following theorem.

Theorem 9.

$$\mathcal{H}(C_{a_k}(C_6), x) = (2 \cdot 3^k + 6)x^3 + 8 \cdot 3^k x^4 + (6 \cdot 7^k - 4 \cdot 3^k - 6)x^5$$

and

$$\mathcal{H}(C_{a_k}(C_6)) = 7^k + \frac{43}{30} \cdot 3^k + \frac{1}{2}.$$

Proof. By analyzing the molecular structure of $C_{a_k}(C_6)$, we observe that the set of edges of $C_{a_k}(C_6)$ can be partitioned into three sets based on the degrees of the vertices, is shown in Table 12.

Table 12. **The edge partition of** $C_{a_k}(C_6)$.

(d_u, d_v)	$(2, 2)$	$(2, 3)$	$(3, 3)$
Number of edges	$3^k + 3$	$4 \cdot 3^k$	$3 \cdot 7^k - 2 \cdot 3^k - 3$

Thus, according to the definition, we will have a harmonic polynomial:

$$\mathcal{H}(C_{a_k}(C_6), x) = (2 \cdot 3^k + 6)x^3 + 8 \cdot 3^k x^4 + (6 \cdot 7^k - 4 \cdot 3^k - 6)x^5$$

and

$$\mathcal{H}(C_{a_k}(C_6)) = 7^k + \frac{43}{30} \cdot 3^k + \frac{1}{2}.$$

□

2.7. Nanocone

A nanocone is derived from a single layer of graphene by removing the blade and connecting the edges, resulting in a cone with a single triangular, square, or pentagonal face at its tip. Let $NC_n(k)$ be an arbitrary nanocone where n denotes the number of edges of triangles, squares, pentagons, and etc. k represents the number of layers. Yang and Hua calculated the harmonic index for nanocones in their paper [13] (see Figure 12).
In the following, we derive a simple formula for the harmonic index and the harmonic polynomial of a nano-cone $NC_n(k)$.

Theorem 10. *If $NC_n(k)$ be the mentioned nanocone, then*

$$\mathcal{H}(NC_n(k), x) = 2nx^3 + 4knx^4 + kn(3k + 1)x^5$$

and

$$\mathcal{H}(NC_n(k)) = \frac{1}{2}n + \frac{29}{30}kn + \frac{1}{2}k^2 n.$$

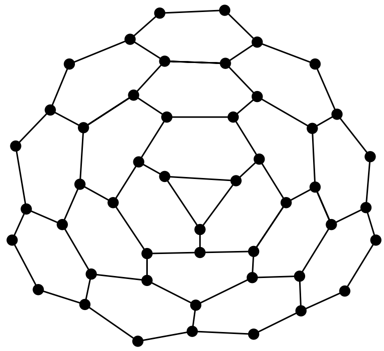

Figure 12. **A nanocone** $NC_3(3)$.

Proof. In the nanocone $NC_n(k)$, there are n edges with endpoints of degree 2. Additionally, there are $2kn$ edges with endpoints of degree 2, 3, and there are $\frac{kn(3k+1)}{2}$ edges with endpoints of degree 3. The partition of the edges of $NC_n(k)$ based on the degrees of the vertices is shown in Table 13.

Table 13. **The edge partition of** $NC_n(k)$.

(d_u, d_v)	$(2,2)$	$(2,3)$	$(3,3)$
Number of edges	n	$2kn$	$\frac{kn(3k+1)}{2}$

Thus, according to the definition, we will have a harmonic polynomial.

$$\mathcal{H}(NC_n(k), x) = 2nx^3 + 4knx^4 + kn(3k+1)x^5$$

and

$$\mathcal{H}(NC_n(k)) = \frac{1}{2}n + \frac{29}{30}kn + \frac{1}{2}k^2n.$$

□

2.8. Spiro chain

Spiro chains refer to a specific type of chain where components or rings are connected in such a way that they intersect at specific points (usually by sharing one or more points), creating a complex and unique structure. Spiro chains are commonly used in organic chemistry and the design of complex molecules. This type of chain can be found in various structures, including drugs and new materials. Dendrimers, graphene, and spiro chains represent different concepts in chemistry and materials

science [14]. A chain of k cycles C_q is denoted by $S_{q,h,k}$, where h represents the distance between two consecutive vertices of the bond.
We denote the chain of k cycles C_q by $S_{q,h,k}$, where h represents the join between two consecutive vertices (see Figures 13 and 14).

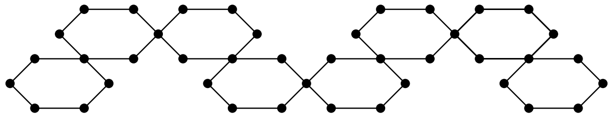

Figure 13. **Graph** $S_{6,2,8}$.

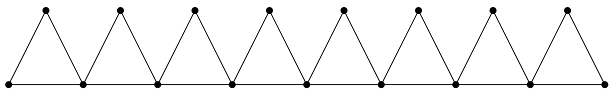

Figure 14. **Graph** $S_{3,1,8}$.

Theorem 11. *Let* $G = S_{q,h,k}$, *then*

$$\mathcal{H}(G,x) = \begin{cases} 2(k-2)x^7 + 4kx^5 + 2(qk-3k+2)x^3, & if \quad h=1 \\ 8(k-1)x^5 + 2(qk-4(k-1))x^3, & if \quad h \geq 2 \end{cases}$$

and

$$\mathcal{H}(G) = \begin{cases} \frac{1}{2} + \frac{1}{2}qk - \frac{7}{12}k, & if \quad h=1 \\ \frac{1}{2}qk - \frac{2}{3}(k-1), & if \quad h \geq 2. \end{cases}$$

Proof. In the graph $S_{q,1,k}$, there are $(k-2)$ edge with endpoints of degree 4. Additionally, there are $2k$ edges with endpoints of degree 2 and 4, and $(qk-3k+2)$ edges with endpoints of degree 2. In the graph $S_{q,h,k}$, there are $4(k-1)$ edges with endpoints of degree 2 and 4. Additionally, there are $(qk-4(k-1))$ edges with endpoints of degree 2. The partition of the edges of G based on the degrees of the vertices is shown in Table 14.

Table 14. **The edge partition of** G.

(d_u, d_v)	$(2,2)$	$(2,4)$	$(4,4)$	$if \quad h=1$
Number of edges	$qk-3k+2$	$2k$	$k-2$	
(d_u, d_v)	$(2,2)$	$(2,4)$	-	$if \quad h \geq 2$
Number of edges	$qk-4(k-1)$	$4(k-1)$	-	

Thus, according to the definition, we will have a harmonic polynomial.

$$\mathcal{H}(G,x)=\begin{cases}2(k-2)x^7+4kx^5+2(qk-3k+2)x^3, & if \quad h=1\\ 8(k-1)x^5+2(qk-4(k-1))x^3, & if \quad h\geq 2\end{cases}$$

and

$$\mathcal{H}(G)=\begin{cases}\frac{1}{2}+\frac{1}{2}qk-\frac{7}{12}k, & if \quad h=1\\ \frac{1}{2}qk-\frac{2}{3}(k-1), & if \quad h\geq 2.\end{cases}$$

□

2.9. Polyphenylenes

Polyphenylene is a type of engineering polymer that has garnered attention among plastic materials due to its superior physical and chemical properties. This polymer is a popular choice in industries such as electronics, automotive, and medical engineering because of its high strength, thermal resistance, and chemical resistance. Additionally, polyphenylene is widely used in the production of electronic components and automotive body parts due to its low thermal conductivity and excellent moisture resistance [12]. Polyphenylene can be defined as a join k of cycle C_q, where h is the distance between two contacting vertices in a cycle (see Figures 15 and 16).

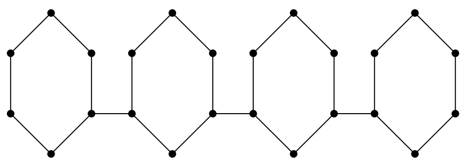

Figure 15. **Graph** $L_{6,2,4}$.

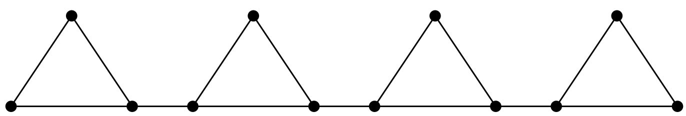

Figure 16. **Graph** $L_{3,1,4}$.

Theorem 12. *Let* $G=L_{q,h,k}$. *Then*

$$\mathcal{H}(G,x)=\begin{cases}2(2k-3)x^5+4kx^4+2(qk-3k+2)x^3, & if \quad h=1\\ 2(k-1)x^5+8(k-1)x^4+2(qk-4(k-1))x^3, & if \quad h\geq 2\end{cases}$$

and

$$\mathcal{H}(G) = \begin{cases} \frac{1}{2}qk - \frac{1}{30}k, & if \quad h = 1 \\ \frac{1}{15} + \frac{1}{2}qk - \frac{1}{15}k, & if \quad h \geq 2. \end{cases}$$

Proof. In the graph $L_{q,1,k}$, there are $(2k-3)$ edges with endpoints of degree 3. Additionally, there are $2k$ edges with endpoints of degree 2 and 3, and $qk-3k+2$ edges with endpoints of degree 2. In the graph $L_{q,h,k}$, there are $k-1$ edges with endpoints of degree 3. Additionally, there are $4(k-1)$ edges with endpoints of degree 2 and 3, and $qk-4(k-1)$ edges with endpoints of degree 2. The partition of the edges of G based on the degrees of the vertices is shown in Table 15

Table 15. **The edge partition of G.**

(d_u, d_v)	$(2,2)$	$(2,3)$	$(3,3)$	$if \quad h=1$
Number of edges	$qk-3k+2$	$2k$	$2k-3$	
(d_u, d_v)	$(2,2)$	$(2,3)$	$(3,3)$	$if \quad h \geq 2$
Number of edges	$qk-4(k-1)$	$4(k-1)$	$k-1$	

Thus, according to the definition, we will have the harmonic polynomial.

$$\mathcal{H}(G,x) = \begin{cases} 2(2k-3)x^5 + 4kx^4 + 2(qk-3k+2)x^3, & if \quad h=1 \\ 2(k-1)x^5 + 8(k-1)x^4 + 2(qk-4(k-1))x^3, & if \quad h \geq 2 \end{cases}$$

and

$$\mathcal{H}(G) = \begin{cases} \frac{1}{2}qk - \frac{1}{30}k, & if \quad h = 1 \\ \frac{1}{15} + \frac{1}{2}qk - \frac{1}{15}k, & if \quad h \geq 2. \end{cases}$$

□

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Data Availability: Data sharing is not applicable to this article as no data sets were generated or analyzed during the current study.

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