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General $(\alpha, 2)$ Path Sum Connectivity Index of Nanostructures

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Abstract

The general path sum connectivity index of a molecular graph, denoted as ${}^t\chi_\alpha(G)$, is defined for a graph G, where α is a positive real number and t is a positive integer. This index is expressed as:

$$ {}^t\chi_\alpha(G) = \sum_{p^t = v_{j_1} v_{j_2} \cdots v_{j_{t+1}} \subseteq G} \left[d_G(v_{j_1}) + d_G(v_{j_2}) + \cdots + d_G(v_{j_{t+1}}) \right]^\alpha , $$

where p^t represents a path of length t within the graph. In this work, we compute the general path sum connectivity index for various nanostructures, including phenylene, naphthalene, anthracene, and tetracene nanotubes. This index is particularly useful in investigating the physico-chemical properties of chemical compounds and plays a crucial role in the analysis of three-dimensional quantitative structure-activity relationships (3D-QSAR) and molecular chirality.

Keywords: graph energy, The general (α, t) path connectivity index, degree based topological index phenylenic, Naphatalenic, Anthracene and Tetracenic nanotubes

1. Introduction

Graph theory is an integral branch of mathematics with widespread applications across various scientific fields, including chemistry, physics, medicine, and engineering. Its relevance is particularly evident in areas that involve complex systems and interactions, where graph models provide a structured framework to analyze relationships and connections. In chemistry, for instance, molecular structures can be effectively modeled as graphs, where atoms represent the vertices and bonds between atoms represent the edges. By leveraging mathematical tools and concepts from graph theory, researchers can gain deeper insights into the behavior and properties of molecules, aiding in the understanding of chemical reactions and molecular stability.

One of the most notable applications of graph theory in chemistry is the use of topological indices or descriptors. These are numerical values derived from the structure of a molecular graph that correlate strongly with various physio-chemical properties of the compounds they represent. Topological indices have been shown to have significant predictive power when it comes to properties such as boiling point, melting point, bond energy, and molecular size. By applying different graph-theoretical approaches, researchers can derive a variety of indices, each of which emphasizes different structural features of the molecular graph. Some of the most widely used indices include the Randic Connectivity Index [1], the Sum Connectivity Index [2, 3], and the first and second Zagreb Indices [4–10].

The Randic Connectivity Index, one of the pioneering topological indices, measures the branching of a molecular structure and is used to predict the molecular stability and reactivity of hydrocarbons. Similarly, the Sum Connectivity Index and the Zagreb Indices provide different perspectives on molecular structure, considering factors such as vertex degrees and edge contributions. These indices are invaluable tools in quantitative structure-property relationships (QSPR) and quantitative structure-activity relationships (QSAR), which are techniques used to predict the properties or activities of chemical compounds based on their molecular structure.

The application of topological indices extends beyond theoretical predictions. In practical terms, they have been instrumental in areas such as drug discovery and the development of new materials. In the pharmaceutical industry, for example, QSAR models that utilize topological indices help researchers identify potential drug candidates by analyzing molecular structures and predicting their biological activities. This approach accelerates the process of drug development by providing a cost-effective and time-efficient method for screening large libraries of compounds.

Additionally, topological indices have been used to predict a range of physio-chemical properties such as enthalpy changes, entropy, and heat capacity, making them essential in fields like thermodynamics and material science. By providing quantitative measures that are invariant under graph isomorphisms, these indices allow researchers to compare and classify

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molecules based on their structural properties, leading to more targeted experiments and innovations in material design. The robustness and versatility of topological indices continue to make them a focal point in the study of molecular graphs.

In this work, we focus on extending the use of graph-theoretical indices by computing the general path sum connectivity index for several nanostructures, including phenylene, naphthalene, anthracene, and tetracene nanotubes. These nanostructures are of particular interest due to their unique properties and applications in nanotechnology, electronics, and materials science. By applying the general path sum connectivity index to these structures, we aim to provide new insights into their physio-chemical properties, contributing to a deeper understanding of their behavior and potential applications in various scientific and industrial domains.

2. Results and Discussion

In graph theory, a graph G is defined by its vertices $V(G)$ and edges $E(G)$. For molecular graphs, atoms are represented by vertices, while chemical bonds are modeled by edges. In 1947, chemist Harold Wiener introduced the Wiener index $W(G)$ [11], which is given by:

$$W(G) = \frac{1}{2} \sum_{u \in V(G)} \sum_{v \in V(G)} d(u, v),$$

where $d(u, v)$ represents the topological distance between any two atoms in the molecular graph. The Wiener index has significant applications in chemistry and was used to analyze trees in [13]. In 1988, Haruo Hosoya introduced the Hosoya polynomial for molecular graphs [12]:

$$H(G, x) = \frac{1}{2} \sum_{u \in V(G)} \sum_{v \in V(G)} x^{d(u,v)}.$$

This polynomial is based on topological distances between vertices. In 2001, the Wiener index of trees was further investigated [13]. Another influential polynomial, introduced by Deutsch and Klavžar in 2015, is the M-polynomial, which plays a crucial role in topological analysis [14]:

$$M(G, x, y) = \sum_{\delta \leq i \leq j \leq \Delta} m_{ij}(G) x^i y^j,$$

where δ and Δ are the minimum and maximum degrees of vertices in G. Additionally, the Zagreb indices, introduced by Gutman and Trinajstić, see [4–10], are defined as follows:

- First Zagreb index $Zg_1(G)$:

$$Zg_1(G) = \sum_{uv \in E(G)} (d_u + d_v).$$

- Second Zagreb index $Zg_2(G)$:

$$Zg_2(G) = \sum_{uv \in E(G)} (d_u \times d_v).$$

In 1975, Milan Randić introduced the Randić Connectivity Index [1], a degree-based molecular descriptor:

$$\chi(G) = \sum_{e=uv \in E(G)} \frac{1}{\sqrt{d_u d_v}}.$$

Its generalized version, introduced by Bollobás and Amic, see [15] is given by:

$$R_\alpha(G) = \sum_{uv \in E(G)} \frac{1}{d_u d_v^\alpha}.$$

The Randić index has widespread applications in drug discovery. The Sum Connectivity Index [2, 3] is defined as:

$$\chi(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_u + d_v}}.$$

This concept was generalized by Wang and introduced the General Sum Connectivity Index [16]:

$$\chi_\alpha(G) = \sum_{uv \in E(G)} [d_G(u) + d_G(v)]^\alpha.$$

Wang further extended this concept to the context of (α, t)-path sum connectivity indices, defined as:

$$ {}^{t}\chi_{\alpha}(G) = \sum_{p^t = v_{j_1} v_{j_2} \ldots v_{j_{t+1}} \subseteq G} \left[d_G(v_{j_1}) + d_G(v_{j_2}) + \cdots + d_G(v_{j_{t+1}}) \right]^{\alpha}. $$

In 2017, M-polynomials and topological indices for V-phenylenic nanotubes and nanotori were investigated in [17]. These compounds, consisting of C_4, C_6, and C_8 nets, have been extensively studied, including vertex P1 indices [18], GA indices [19], and eccentricity indices [20]. In March 2019, Sunantha et al. [21] proposed degree-based multiplicative connectivity indices for nanostructures. In this work, we compute the α, t-general path sum connectivity index for various nanotubes such as phenylenic, naphthalene, anthracene, and tetracene, which are highly relevant in the field of nanotechnology.

2.1 Results for V-phenylenic Nanotube

The V-phenylenic nanotube is denoted by $VPHX(m, n)$, where m and n represent the number of hexagons in the first row and first column, respectively.

Lemma 2.1. *There are two types of vertices with degrees 2 and 3 in $VPHX(m, n)$. The vertex and edge cardinalities are given by:*

$$ |V(H_1)| = 6mn, \quad |E(H_1)| = 9mn - m. $$

The vertex set of H_1 is partitioned into two subsets: one containing edges m_{23} (connecting vertices of degrees 2 and 3) and the other containing edges m_{33} (connecting vertices of degree 3).

Degree of Vertices	Number of Vertices	Type of Edge	Number of Edges
2	$2m$	$(2,3)$	$4m$
3	$6mn - 2m$	$(3,3)$	$9mn - 5m$

Table 1: Vertex and edge partition details of $VPHX(m, n)$

Theorem 2.2. *For any real number α, the general $(\alpha, 2)$-path sum connectivity index of $VPHX(m, n)$ is given by:*

$$ \chi^2_{\alpha}(VPHX(m, n)) = 2m \left[9n \times 3^{2\alpha} + 5 \times 2^{3\alpha} + 7 \times 3^{2\alpha} \right]. $$

Proof. There are two types of edges in $VPHX(m, n)$: $(2, 3)$-edges and $(3, 3)$-edges. First, we calculate the total number of possible 2-paths, represented by $N(p^2)$. For any $(2, 3)$-edge, there are 3 different paths containing this edge. With $4m$ such edges, the total number of 2-paths containing this edge is $4m \times 3 = 12m$. Similarly, for any $(3, 3)$-edge, there are 4 different paths containing this edge, and with $m(9n - 5)$ such edges, the total number of 2-paths is $4 \times m(9n - 5)$.

By calculating and combining the paths, we derive the expression for $\chi^2_{\alpha}(VPHX(m, n))$. □

Theorem 2.3. *For V-phenylenic nanotube $VPHX(m, n)$, the general sum connectivity index $\chi^2_{\alpha}(VPHX(m, n))$ is strictly increasing with respect to positive integers m and n, and for any real number α.*

Proof. It is clear that $\chi^2_{\alpha}(VPHX(m, n))$ is strictly increasing with respect to m and n. By increasing m and n, the value of the index increases. □

Theorem 2.4. *For V-Naphatalanic Nanotubes, $NPHX(m, n)$, the general sum connectivity index ${}^{2}\chi_{\alpha}(m, n)$ is strictly increasing with respect to positive integers m and n for any real number α.*

Proof. Let us find the values of m and n where the value of ${}^{2}\chi_{\alpha}(NPHX(m, n)) = 0$.

$$ 2m[7^{\alpha} + (8)^{\alpha+1} + (15n - 13)9^{\alpha}] = 0 $$

so, $m = 0$, and

$$ 9\alpha[15n - 13 + \frac{7\alpha + 8^{\alpha+1}}{9^{\alpha}}] = 0 $$

$$ 15n = 13 - \frac{7^{\alpha} + (8)^{\alpha+1}}{9^{\alpha}} $$

$$ n = \frac{13}{15} - \frac{7^{\alpha} + (8)^{\alpha+1}}{15 \cdot 9^{\alpha}} $$

$$ n = \frac{13}{15} \left(1 - \frac{1}{13} \cdot \frac{7^{\alpha} + (8)^{\alpha+1}}{9^{\alpha}} \right). $$

Degree of Vertices	Number of Vertices	Type of Edge	No of Edges
2	$6m$	$(2,3)$	$12m$
3	$14mn-6m$	$(3,3)$	$21mn-15m$

Table 2: Table 3: Vertex and edge partition of $ATHX(m,n)$.

Since $n < \frac{13}{15}$, but n is a positive integer, $n = 0$. Hence, at $m = 0$ and $n = 0$, this index vanishes, which shows that ${}^2\chi_\alpha(NPHX(m,n))$ is strictly increasing with m and n. Its minimum value is obtained by setting $m = n = 2$, and this minimum value is

$$4[7^\alpha + (8)^{\alpha+1} + 17 \cdot 9^\alpha].$$

□

3. Results for V-Anthracene Nanotubes (V_A)

Let this structure be represented by $ATHX(m,n) = H_3$, where m and n represent the number of pairs of hexagons in the first row and column, respectively.

Lemma 3.1. *The total number of vertices is* $14mn$*, and the total number of edges is* $21mn - 3m$ *in* $ATHX(m,n)$*, where* $m, n > 1$*.*

Theorem 3.2. *For any real number* α*, the general* $(\alpha,2)$*-path sum connectivity index of* $ATHX(m,n)$ *is given by*

$${}^2\chi_\alpha(ATHX(m,n)) = 2m[11(8^\alpha) + 2(7)^\alpha + (21n-19)9^\alpha].$$

Proof. There are two types of edges in $ATHX(m,n)$: $(2,3)$ edge e and $(3,3)$ edge e'. First, we calculate the total number of possible 2-paths, represented by $N(p^2)$. Consider any $(2,3)$ edge e. As per the structure of $ATHX(m,n)$, there are 3 different paths containing this edge. Since there are $12m$ such edges, we conclude there are $12 \times 3 = 36m$ such 2-paths containing this edge.

Next, take any $(3,3)$ edge e'. By analyzing the structure of $ATHX(m,n)$, we find that there are 4 paths containing this edge. Since there are $(21mn - 15m)$ such edges, in total there are $4 \times (21mn - 15m)$ such 2-paths. Since the paths $V_{j_1}V_{j_2} - -V_{j_{t+1}}$ and $V_{j_{t+1}}...V_{j_2}V_{j_1}$ represent identical paths, such paths are counted twice. Thus,

$$\begin{aligned} N(p^2) &= \frac{4 \times (21mn-15m) + 3 \times 12m}{2} \\ &= \frac{84mn-24m}{2} \\ &= 42mn - 12m. \end{aligned}$$

There are four possible degree sequences of 2-edge paths: $(2,3,3)$, $(3,2,3)$, $(3,3,3)$, and $(2,3,2)$. We calculate $P_{233} + P_{323} + P_{333} + P_{232} = N(p^2)$, where P_{abc} represents the number of two-edge paths passing through vertices of degrees a, b, and c.

For the path sequence $(2,3,3)$, which begins or ends with a vertex of degree 2, there are $6m$ such vertices. Out of these, $4m$ vertices produce 3 different paths, and $2m$ vertices produce 2 different paths. Thus, there are $P_{233} = 16m$ such paths. Similarly, $P_{232} = 4m$, and $P_{323} = 6m$.

Finally, the number of paths with the degree sequence $(3,3,3)$ is given by:

$$\begin{aligned} P_{333} &= N(p^2) - (P_{233} + P_{323} + P_{232}) \\ &= 42mn - 12m - (16m + 4m + 6m) \\ &= 42mn - 38m. \end{aligned}$$

By the definition of the general $(\alpha,2)$-path sum connectivity index,

$$\begin{aligned} {}^2\chi_\alpha(ATHX(m,n)) &= \sum_{P^2=V_{j_1}V_{j_2}V_{j_3}\subseteq H_3} (d_{H_3}(V_{j_1}) + d_{H_3}(V_{j_2}) + d_{H_3}(V_{j_3}))^\alpha \\ &= P_{232}(2+3+2)^\alpha + P_{233}(2+3+3)^\alpha + P_{323}(3+2+3)^\alpha + P_{333}(3+3+3)^\alpha \\ &= 4m(7)^\alpha + 16m(8)^\alpha + 6m(8)^\alpha + (42mn-38m)9^\alpha \\ &= 4m(7)^\alpha + 22m(8)^\alpha + (42mn-38m)9^\alpha \\ &= 2m[11(8)^\alpha + 2(7)^\alpha + (21n-19)9^\alpha]. \end{aligned}$$

□

Theorem 3.3. *For V-Anthracene Nanotubes (V_A), the general sum connectivity index ${}^2\chi_\alpha(ATHX(m,n))$ is strictly increasing with respect to positive integers m and n for any real number α.*

Proof. Let us find the values of m and n where the value of ${}^2\chi_\alpha(ATHX(m,n)) = 0$.

$$2m[11(8)^\alpha + 2(7)^\alpha + (21n - 19)9^\alpha] = 0$$

so, $m = 0$, and

$$21n = 19 - \frac{2(7)^\alpha + 11(8)^\alpha}{9^\alpha},$$

$$n = \frac{19}{21} - \frac{2(7)^\alpha + 11(8)^\alpha}{21 \cdot 9^\alpha}.$$

Since $n < \frac{19}{21}$, but n is a positive integer, $n = 0$. Hence, at $m = 0$ and $n = 0$, this index vanishes, which shows that ${}^2\chi_\alpha(ATHX(m,n))$ is strictly increasing with m and n. Its minimum value is obtained by setting $m = n = 2$, and this minimum value is

$$4[11(8)^\alpha + 2(7)^\alpha + 23(9)^\alpha].$$

□

4. Conclusion

In this work, we studied the general $(\alpha, 2)$-path sum connectivity index for some nanostructures, and derived their respective formulas. These results can facilitate investigations in nanoscience, pharmacy, and biochemistry.

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