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General $(\alpha, 2)$-Path Sum-Connectivirty Indices of One Important Class of Polycyclic Aromatic Hydrocarbons

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Received: 14 August 2018; Accepted: 6 September 2018; Published: 21 September 2018

Abstract: The general (α, t)-path sum-connectivity index of a molecular graph originates from many practical problems, such as the three-dimensional quantitative structure–activity relationships (3D QSAR) and molecular chirality. For arbitrary nonzero real number α and arbitrary positive integer t, it is defined as ${}^{t}\chi_{\alpha}(G) = \sum_{P^t=v_{i_1}v_{i_2}\cdots v_{i_{t+1}}\subseteq G}[d_G(v_{i_1})d_G(v_{i_2})\cdots d_G(v_{i_{t+1}})]^{\alpha}$, where we take the sum over all possible paths of length t of G and two paths $v_{i_1}v_{i_2}\cdots v_{i_{t+1}}$ and $v_{i_{t+1}}\cdots v_{i_2}v_{i_1}$ are considered to be one path. In this work, one important class of polycyclic aromatic hydrocarbons and their structures are firstly considered, which play a role in organic materials and medical sciences. We try to compute the exact general $(\alpha, 2)$-path sum-connectivity indices of these hydrocarbon systems. Furthermore, we exactly derive the monotonicity and the extremal values of these polycyclic aromatic hydrocarbons for any real number α. These valuable results could produce strong guiding significance to these applied sciences.

Keywords: topological indices; general (α, t)-path sum-connectivity index; polycyclic aromatic hydrocarbons

1. Introduction

1.1. Application Background

In many fields (e.g., physics, chemistry, and electrical networks), the boiling point, the melting point, the chemical bonds, and the bond energy are all important quantifiable parameters. To understand the physico-chemical properties of chemical compounds or network structures, we abstractly define different concepts, collectively named the topological descriptors or the topological indices after mathematical modelings. We called them different names, such as Randić index and Zagreb index [1–3]. Different index represents its corresponding chemical structures in graph-theoretical terms via arbitrary molecular graph.

In the past decades, these two-dimensional topological indices have been used as a powerful approach to discover many new drugs, such as anticonvulsants, anineoplastics, antimalarials, and antiallergics and Silico generation [4–8]. Therefore, the practice has proven that the topological indices and the quantitative structure-activity relationships (QSAR) have moved from an attractive possibility to representing a foundation stone in the process of drug discovery and other research areas [9–12].

Most importantly, with the further study of chemical indices and drug design and discovery, three-dimensional molecular features (topographic indices) and molecular chirality are also presented. It is increasingly urgent to study the three-dimensional quantitative structure-activity relationships such as molecular chirality. However, so far there have been few results, except for one related definition that is mentioned generally in [8].

1.2. Definitions and Notations

In the whole paper, we always let $G = (V_G, E_G)$ be a simple molecular graph, in which V_G and E_G are the vertex set and edge set of G, respectively. We denote $|V_G|$ and $|E_G|$ as the numbers of vertices and edges of G, respectively. In physico-chemical graph theory, the atoms and the bonds represent the vertices and edges, respectively. Two vertices are called adjacent if there is an edge between them in G. For any vertex $u \in V_G$, the number of its adjacent vertices is called its degree in G and denote $d_G(u)$. The set of all neighbors of u is denoted by $N_G(u)$, and a vertex of G is called a pendant if its degree is 1. Similarly, the minimum and maximum degree of G are denoted by δ_G and Δ_G, respectively. All other notations and terminologies are referred to [13].

In 1975, Randić index was introduced by the chemist M. Randić during his study of alkanes [1]. As a molecular structure-descriptor and a graphical description of molecular structure, Randić index is most commonly used in the quantitative structure-property and structure-activity studies [6,14]. Randić index is defined as the sum over all edges $uv \in E_G$ of a molecular graph of the terms $[d_G(u)d_G(v)]^{-\frac{1}{2}}$. That is,

$$R(G) = \sum_{uv \in E_G} [d_G(u)d_G(v)]^{-\frac{1}{2}}.$$

The first Zagreb index was introduced more than forty years ago by Gutman and Trinajestić [15,16], and is defined as

$$M_1(G) = \sum_{x \in V_G} d_G(x) = \sum_{uv \in E_G} [d_G(u) + d_G(v)].$$

Later [17], some researchers began to define another new index of a graph G as

$$\chi(G) = \sum_{uv \in E_G} [d_G(u) + d_G(v)]^{-\frac{1}{2}},$$

which is named the sum-connectivity index and denoted by $\chi(G)$.

In 2008, Zhou and Trinajestic [17] proposed the sum-connectivity index, which is a closely related variant of Randić connectivity index of G. Now we define the general sum-connectivity index $\chi_\alpha(G)$ as

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

With the intention of extending the applicability of the general sum-connectivity index, we begin to consider the general (α, t)-path sum-connectivity index of G as where we take the sum over all possible paths of length t of G:

$${}^t\chi_\alpha(G) = \sum_{P^t = v_{i_1}v_{i_2}\cdots v_{i_{t+1}} \subseteq G} [d_G(v_{i_1}) + d_G(v_{i_2}) + \cdots + d_G(v_{i_{t+1}})]^{\alpha},$$

with any nonzero real number α and any positive integer t, and two paths $v_{i_1}v_{i_2}\cdots v_{i_{t+1}}$ and $v_{i_{t+1}}\cdots v_{i_2}v_{i_1}$ are considered to be one path.

According to the above definition, the *general* (α, t)*-path sum-connectivity index* of an arbitrary graph is one real constant and an important invariant under graph automorphism. It is closely related to the structures of a molecular graph. For any molecular material, only by mastering its structure can we calculate the exact value of its *general* (α, t)*-path sum-connectivity index*.

In this work, one important class of polycyclic aromatic hydrocarbons and their structures are considered which play a role in organic materials and medical sciences. Then, we try to compute the exact general $(\alpha, 2)$-path sum-connectivity indices of these hydrocarbon systems. Furthermore,

we exactly derive its monotonicity and extremal values for these polycyclic aromatic hydrocarbons for any real number α. These valuable results could produce strong guiding significance to these applied sciences.

For convenience, it is necessary to simplify some basic concepts and notations in polycyclic aromatic hydrocarbons. A vertex with degree i is called an i-vertex. An edge between a j-vertex and a k-vertex is called a (j,k)-edge. Besides, the numbers of i-vertices and (j,k)-edges are denoted as n_i and m_{jk}, respectively.

Let $v_{i_0}v_{i_1}\cdots v_{i_t}$ be a path P^t of length t in polycyclic aromatic hydrocarbons, denoted $P^t = v_{i_0}v_{i_1}\cdots v_{i_t}$. $(d_G(v_{i_0}), d_G(v_{i_1}), \cdots, d_G(v_{i_t}))$ is called its degree sequence. Obviously, there are in total two types (i.e., $(1,3,3)$ and $(3,3,3)$) of degree sequences of different 2-paths in these polycyclic aromatic hydrocarbons in Figure 1. Let m_{133} and m_{333} denote the numbers of all 2-paths of the degree sequence types $(1,3,3)$ and $(3,3,3)$ in polycyclic aromatic hydrocarbons, respectively.

2. Polycyclic Aromatic Hydrocarbons

Polycyclic aromatic hydrocarbons are important and ubiquitous combustion materials. They belong to one class of hydrocarbon molecules. Polycyclic aromatic hydrocarbons have been considered as an important class of carcinogens. They also play a role in the graphitisation of medical science and organic materials [18,19].

In the field of chemical materials, polycyclic aromatic hydrocarbons have become molecular analogues of graphite for interstellar species and building blocks of functional materials for device applications [20–22]. Thus, detailed descriptions of all these molecular properties are necessary for the available synthetic routes to polycyclic aromatic hydrocarbons and their specific applications.

In essence, polycyclic aromatic hydrocarbons can be considered as small pieces of graphene sheets, in which the free valences of the dangling bonds are saturated by hydrocarbons. Vice versa, a graphene sheet can be interpreted as an infinite polycyclic aromatic hydrocarbon molecule [22]. Many scientists have reported many successful applications of polycyclic aromatic hydrocarbons in graphite surface modeling. As we know, *benzenoid systems* are a very famous family of hydrocarbon molecules and belong to the *circumcoronene homologous series* of *benzenoid*, and polycyclic aromatic hydrocarbons have very similar properties to them.

One important class of polycyclic aromatic hydrocarbons shown in Figure 1 belong to linear and regular circular polycyclic aromatic hydrocarbons [22]. However, the class of *symmetrical poly-aromatic hydrocarbons* is important in sciencesw. For an arbitrary positive integer n, let PAH_n be the general expression of this class of polycyclic aromatic hydrocarbons shown in Figure 1.

Obviously, the first three members of this hydrocarbon family are given in Figure 2, where PAH_1 is called *benzene*, PAH_2 *coronene*, and PAH_3 *circumcoronene* . Obviously, *benzene* has 6 carbon atoms and 6 hydrogen atoms, *coronene* has 24 carbon atoms and 12 hydrogen atoms, and *circumcoronene* has 54 carbon atoms and 18 hydrogen atoms.

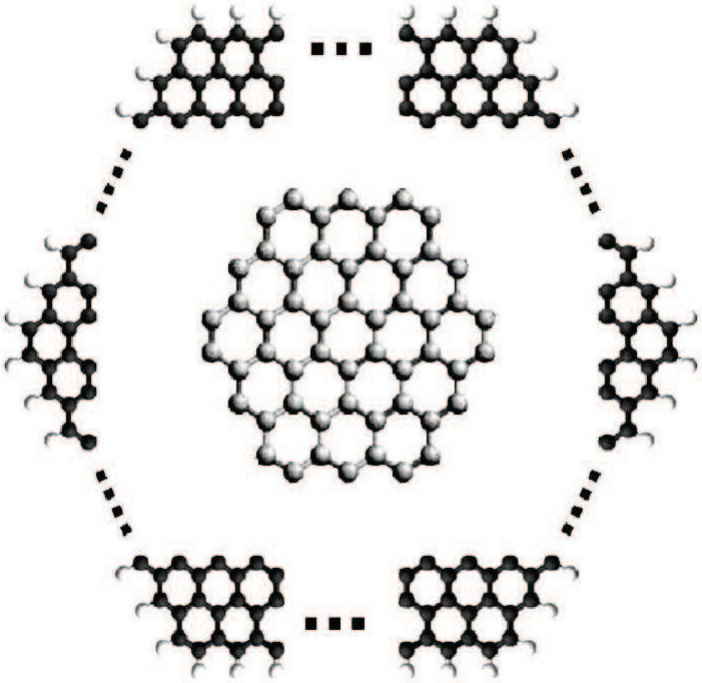

Figure 1. General representation of a polycyclic aromatic hydrocarbon.

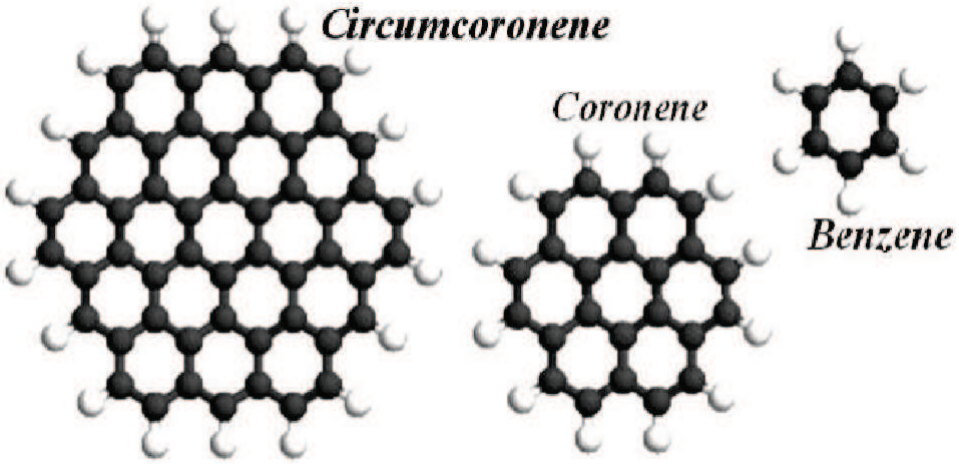

Figure 2. The first three graphs of polycyclic aromatic hydrocarbons.

From Figure 1 above, we know that the class *polycyclic aromatic hydrocarbon* PAH_n contains $6n^2$ carbon atoms and $6n$ are hydrogen atoms. Thus, this molecular graph has $6n^2 + 6n$ vertices or atoms such that $6n^2$ of them are carbon atoms and $6n$ are hydrogen atoms. Each hydrogen atom is 1-vertex and each carbon atom is 3-vertex in PAH_n. Therefore, this hydrocarbon molecule PAH_n satisfies that $|V_{PAH_n}| = 6n^2 + 6n$. In this hydrocarbon molecule, we have

$$|E_{PAH_n}| = \frac{3 \times 6n^2 + 1 \times 6n}{2} = 9n^2 + 3n,$$

in which $|E_{PAH_n}|$ means its number of edges (actually chemical bonds).

According to Figure 1, each hydrogen atoms has just one edge/bond between only one carbon atom in the class of polycyclic aromatic hydrocarbon system. Any other carbon atoms just have three bonds with carbon atoms or hydrogen atoms. From the structure of Figure 1, it is clear that we can

divide the edge set of the class of polycyclic aromatic hydrocarbons into two partitions: the $(1,3)$-edge subset and the $(3,3)$-edge subset. Thus,

$$m_{13} = n_1 = 6n$$

and

$$m_{33} = |E_{PAH_n}| - n_1 = 9n^2 - 3n.$$

3. Main Results on the General $(\alpha, 2)$-Path Sum-Connectivity Indices of PAH_n

In this section, let PAH_n be the general representation of the class of polycyclic aromatic hydrocarbon molecules in Figure 1 for any positive integer n. Then, there are $6n$ hydrogen atoms and $6n^2$ carbon atoms in PAH_n. We compute *the general* $(\alpha, 2)$*-path sum-connectivity index* of a family of polycyclic aromatic hydrocarbons as follows. The indices should directly reflect the material's natural properties.

Theorem 1. *For an arbitrary real number* α*, the general* $(\alpha, 2)$*-path sum-connectivity index of* PAH_n *is equal to*

$$^2\chi_\alpha(PAH_n) = 6 \cdot n \cdot [3^{2\alpha+1} \cdot n - 2(9^\alpha - 7^\alpha)]. \quad (1)$$

Proof of Theorem 1. According to the structures of PAH_n, consider any $(1,3)$-edge e. Then, there are in total two different 2-paths, and each path contains this edge e. Consider any $(3,3)$-edge e'. There are in total four different 2-paths, and each path contains this edge e'. Since we do not distinguish between the paths $v_{i_1}v_{i_2}\cdots v_{i_{t+1}}$ and $v_{i_{t+1}}\cdots v_{i_2}v_{i_1}$, each 2-path of PAH_n will compute twice. Then, the total number of different 2-paths, denoted $N(P^2)$, is

$$N(P^2) = \frac{N_H \cdot 2 + m_{33} \cdot 4}{2} = \frac{6n \cdot 2 + (9n^2 - 3n) \cdot 4}{2} = 18n^2.$$

□

If the degree sequence of a 2-path is the type $(1,3,3)$, then this path begins or ends with one hydrogen atom. Obviously, each hydrogen atom can produce two different P^2, and there are $6n$ hydrogen atoms in PAH_n. Then,

$$m_{133} = 2 \cdot m_{13} = 2 \cdot 6n = 12n.$$

Since there are in total two types $(1,3,3)$ and $(3,3,3)$ of degree sequences of 2-paths in PAH_n, we have

$$m_{333} + m_{133} = N(P^2),$$

which induces that

$$m_{333} = N(P^2) - m_{133} = 18n^2 - 12n.$$

By usage of the definitions of *the general* $(\alpha, 2)$*-path sum-connectivity index*, we can compute it of the polycyclic aromatic hydrocarbon in Figure 1 as follows:

$$^2\chi_\alpha(PAH_n) = \sum_{P^2 = v_{i_1}v_{i_2}v_{i_3} \in G} [d_G(v_{i_1}) + d_G(v_{i_1}) + d_G(v_{i_1})]^\alpha$$

$$= m_{133} \cdot (1+3+3)^\alpha + m_{333} \cdot (3+3+3)^\alpha$$

$$= (12n) \cdot 7^\alpha + (18n^2 - 12n) \cdot 9^\alpha$$

$$= 6 \cdot n \cdot [3^{2\alpha+1} \cdot n - 2(9^{\alpha} - 7^{\alpha})].$$

4. The Monotonicity and the Extremal Values of ${}^2\chi_\alpha(PAH_n)$

Let PAH_n be the general representation of the class of polycyclic aromatic hydrocarbon molecules shown in Figure 1 for any positive integer n. In this section, we approach the monotonicity and the extremal values of ${}^2\chi_\alpha(PAH_n)$ for any real number α.

By Equation (1), we can see that ${}^2\chi_\alpha(PAH_n)$ is a strictly increasing function on n. That is, the larger n is, the larger ${}^2\chi_\alpha(PAH_n)$ is.

Let

$$ {}^2\chi_\alpha(PAH_n) = 6 \cdot n \cdot [3^{2\alpha+1} \cdot n - 2(9^{\alpha} - 7^{\alpha})] = 0. \quad (2)$$

Then, Equation (2) has two real zeroes $n_1 = 0$ and $n_2 = \frac{2}{3}[1 - (\frac{7}{9})^{\alpha}]$.

It is clear that

$$n_2 = \frac{2}{3}[1 - (\frac{7}{9})^{\alpha}] < \frac{2}{3}$$

for any real number α. Thus, ${}^2\chi_\alpha(PAH_n)$ is a strictly increasing function on the positive number n and for any real number α.

Thus, we can conclude the theorem as follows.

Theorem 2. *Let PAH_n be the general representation of the class of polycyclic aromatic hydrocarbon molecules shown in Figure 1. Then*

1. *For any real number α, we have ${}^2\chi_\alpha(PAH_n)$ is strictly increasing with respect to all positive integers n.*
2. *The smallest general $(\alpha, 2)$-path sum-connectivity index of Polycyclic aromatic hydrocarbons is*

$$ {}^2\chi_\alpha(PAH_n)_{min} = {}^2\chi_\alpha(PAH_1) = 6[9^{\alpha} + 2 \cdot 7^{\alpha}] \quad (3)$$

when and only when $n = 1$. Of course, PAH_1 is benzene (see Figure 1).

5. Conclusions

The general sum-connectivity index $\chi_\alpha(PAH_n)$ and its minimum value of the class of polycyclic aromatic hydrocarbons can be obtained by substituting the specific value $t = 1$ in the results above.

6. Further Research

In this article, we only consider one important class of *symmetrical poly-aromatic hydrocarbons* PAH_n (see Figure 1), which belong to linear and regular circular polycyclic aromatic hydrocarbons [22]. However, there are broader and more useful polycyclic aromatic hydrocarbons in the world. There are many linearly fused circular *PAHs* with different structures, such as *naphthalene*, *anthracene*, *tetracene*, and *pentacene*. On the other hand, there are great nonlinear and irregular or non-symmetrical aromatic hydrocarbons, such as *pyrene*, *benzopyrene*, derivatives of *azulene* and *pentahelicene*. In the future, we intend to conduct scientific research on the relationship between the complicated aromatic hydrocarbons and their *general* (α, t)*-path sum-connectivity indices*. This research will be very meaningful, interesting and worthwhile.

Funding: This research was funded by National Science Foundation of China [No. 11701530] and Fundamental Research Funds for the Central Universities [No. 2652015193] and [No. 2652017146].

Acknowledgments: The author is indebted to Assistant Editor Jocelyn He and the anonymous referees for their valuable comments and remarks that improved the presentation of the paper.

Conflicts of Interest: The author declares no conflict of interest.

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