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Research Article

General Randić, Sum-Connectivity, Hyper-Zagreb and Harmonic Indices, and Harmonic Polynomial of Molecular Graphs

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We present explicit formula for the general Randić connectivity, general sum-connectivity, Hyper-Zagreb and Harmonic Indices, and Harmonic polynomial of some simple connected molecular graphs.

1. Introduction

In this paper, we consider only simple connected graphs without loops and multiple edges. A connected graph is a graph such that there is a path between all pairs of vertices. Let $G = (V, E)$ be an arbitrary simple connected graph; we denote the vertex set and the edge set of G by $V(G)$ and $E(G)$, respectively. For two vertices u and v of $V(G)$, the distance between u and v is denoted by $d(u, v)$ and defined as the length of any shortest path connecting u and v in G. For a vertex v of $V(G)$, the degree of v is denoted by d_v and is the number of vertices of G adjacent to v.

In chemical graph theory, we have many invariant polynomials and topological indices for a molecular graph. A topological index is a numerical value for correlation of chemical structure with various physical properties, chemical reactivity, or biological activity [1–3].

One of the oldest topological indices or molecular descriptors is the Zagreb index that has been introduced more than forty years ago by Gutman and Trinajstić in 1972 [4].

Now, we know that, for a molecular graph $G = (V, E)$, the first Zagreb index $M_1(G)$ and the second Zagreb index $M_2(G)$ are defined as

$$M_1(G) = \sum_{v \in V(G)} (d_v)^2,$$
$$\text{or } M_1(G) = \sum_{e=uv \in E(G)} (d_u + d_v), \tag{1}$$
$$M_2(G) = \sum_{e=uv \in E(G)} (d_u \times d_v).$$

Recently, a new version of Zagreb indices named Hyper-Zagreb index was introduced by Shirdel et al. in 2013 [5] and it is defined as

$$HM(G) = \sum_{e=uv \in E(G)} (d_u + d_v)^2. \tag{2}$$

We encourage the reader to consult [6–30] for historical background and mathematical properties of the Zagreb indices.

In 1975, Randić proposed a structural descriptor called the branching index [31] that later became the well-known Randić molecular connectivity index. Motivated by the definition of Randić connectivity index based on the end-vertex degrees of edges in a graph defined as the sum of the weights $(d_u d_v)^{-1/2}$ of all edges uv of G,

$$R(G) = \sum_{e=uv \in E(G)} \frac{1}{\sqrt{d_u d_v}}. \tag{3}$$

Later, the Randić connectivity index had been extended as the general Randić connectivity index, which is defined as the sum of the weights $(d_u d_v)^{\alpha}$ $(\forall \alpha \in \mathbb{Q})$ and is equal to

$$R^{\alpha}(G) = \sum_{e=uv \in E(G)} (d_u d_v)^{\alpha}. \tag{4}$$

Also, a closely related variant of Randić connectivity index called the sum-connectivity index was introduced by Zhou and Trinajstić in 2008 [32, 33]. The sum-connectivity index $X(G)$ is defined as

$$X(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_u + d_v}}. \tag{5}$$

The general sum-connectivity index of a graph G is equal to $(\forall \alpha \in \mathbb{Q})$

$$X^{\alpha}(G) = \sum_{e=uv \in E(G)} (d_u + d_v)^{\alpha}. \tag{6}$$

In 1987 [34], Fajtlowicz introduced the Harmonic index $H(G)$ of a graph G which is defined as the sum of the weights $2(d_u d_v)^{-1}$ of $\forall uv \in G$ and is equal to

$$H(G) = \sum_{e=uv \in E(G)} \frac{2}{d_u + d_v}. \tag{7}$$

The Harmonic index is one of the most important indices in chemical and mathematical fields. It is a variant of the Randić index which is the most successful molecular descriptor in structure-property and structure activity relationships studies. The Harmonic index gives somewhat better correlations with physical and chemical properties compared with the well-known Randić index. Estimating bounds for $H(G)$ is of great interest, and many results have been obtained. For example, Favaron et al. [35] considered the relationship between the Harmonic index and the eigenvalues of graphs, and Zhong [36–38] determined the minimum and maximum values of the Harmonic index for simple connected graphs, trees, unicyclic graphs, and bicyclic graphs and characterized the corresponding extremal graphs, respectively. It turns out that trees with maximum and minimum Harmonic index are the path P_n and the star S_n, respectively.

Recently, Iranmanesh and Salehi [39] introduced the Harmonic polynomial $H(G, x)$ of a graph G which is equal to

$$H(G, x) = \sum_{e=uv \in E(G)} 2x^{(d_v + d_v - 1)}, \tag{8}$$

where $H(G) = \int_0^1 H(G, x)dx$.

We encourage the reader to consult [40–43] for more history and mathematical properties of the Randić index and the Harmonic index.

In this paper, we present explicit formula for the general Randić connectivity, general sum-connectivity, Hyper-Zagreb and Harmonic Indices, and Harmonic polynomial of some hydrocarbon molecular graphs.

2. Results and Discussion

In this section, we compute the general Randić connectivity, general sum-connectivity indices, the Hyper-Zagreb and Harmonic Indices, and Harmonic polynomial of a family of hydrocarbon molecules, which are called Polycyclic Aromatic Hydrocarbons PAH_k $(\forall k \in \mathbb{N})$.

The Polycyclic Aromatic Hydrocarbons PAH_k is a family of hydrocarbon molecules, such that its structure is consisting of cycles with length six (benzene). The Polycyclic Aromatic Hydrocarbons can be thought of as small pieces of graphene sheets with the free valences of the dangling bonds saturated by H. Vice versa, a graphene sheet can be interpreted as an infinite PAH molecule. Successful utilization of PAH molecules in modeling graphite surfaces has been reported earlier [44–52] and references therein. Some first members and a general representation of this hydrocarbon molecular family are shown in Figures 1 and 2.

Theorem 1 (see [45]). *Consider the Polycyclic Aromatic Hydrocarbons* PAH_k $(\forall k \in \mathbb{N})$. *Then, the first and second Zagreb indices of* PAH_k *are equal to*

$$\begin{aligned} M_1(PAH_k) &= 54k^2 + 6k, \\ M_1(PAH_k) &= 81k^2 - 3k. \end{aligned} \tag{9}$$

Theorem 2. *The Hyper-Zagreb index of Polycyclic Aromatic Hydrocarbons* PAH_k $(\forall k \in \mathbb{N})$ *is equal to*

$$HM(\mathrm{PAH}_k) = 12k(27k - 1). \tag{10}$$

Theorem 3 (see [46]). *The Randić connectivity and sum-connectivity indices of the Polycyclic Aromatic Hydrocarbons* PAH_k $(\forall k \in \mathbb{N})$ *are equal to*

$$\begin{aligned} R(PAH_k) &= 3k2 + \left(2\sqrt{3} - 1\right)k, \\ X(PAH_k) &= \frac{n}{2}\left(3\sqrt{6}n + 6 - \sqrt{6}\right). \end{aligned} \tag{11}$$

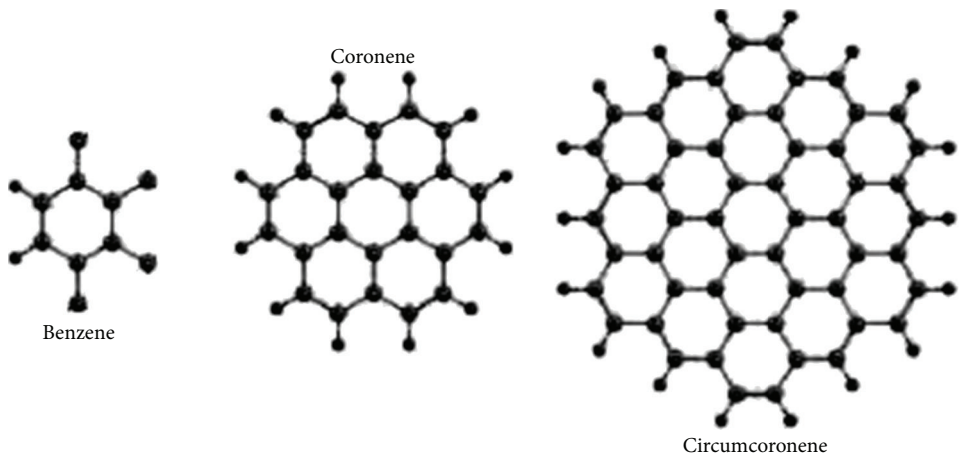

Figure 1: Some first members of the Polycyclic Aromatic Hydrocarbons (PAH_k).

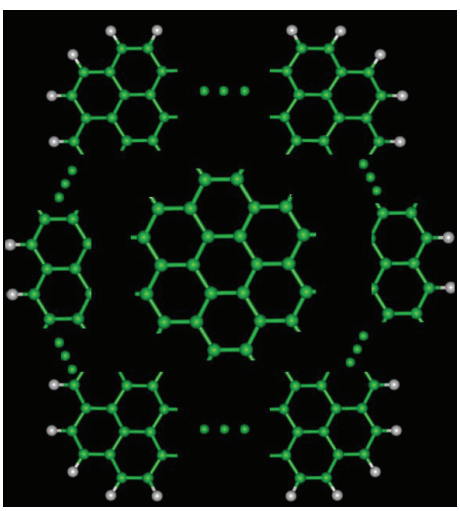

Figure 2: A general representation of the hydrocarbon molecular family "Polycyclic Aromatic Hydrocarbons, PAH_k".

Theorem 4. *Let* PAH_k *be the Polycyclic Aromatic Hydrocarbons. Then,*

(i) *the general Randić connectivity index of* PAH_k *is equal to*

$$R^{\alpha}(PAH_k) = 3k\left(3^{2\alpha+1}k + 3^{\alpha}(2-3^{\alpha})\right), \tag{12}$$

(ii) *the general sum-connectivity index of* PAH_k *is equal to*

$$X^{\alpha}(PAH_k) = 2^{\alpha}3k\left(3^{\alpha+1}k - 3^{\alpha} + 2^{\alpha+1}\right). \tag{13}$$

Theorem 5. *Consider the Polycyclic Aromatic Hydrocarbons* PAH_k. *Then,*

(i) *the Harmonic index of* PAH_k *is equal to* $\forall k \in \mathbb{N}$:

$$H(PAH_k) = 3k^2 + 2k, \tag{14}$$

(ii) *the Harmonic polynomial of* PAH_k *is equal to* $\forall k \in \mathbb{N}$:

$$H(PAH_k, x) = 12kx^3 + 6k(3k-1)x^5. \tag{15}$$

Before presenting the main results, consider the following definition.

Definition 6 (see [10]). Let G be a simple connected molecular graph. We divide the vertex set $V(G)$ and edge set $E(G)$ of G based on the degrees d_v of a vertex/atom v in G. Obviously, $1 \le d_v \le n-1$ and we denote the minimum and maximum of the d_v by δ and Δ, respectively:

$$\begin{aligned} V_k &= \{v \in V(G) \mid d_v = k\} \quad \forall k : \delta \le k \le \Delta, \\ E_i &= \{e = uv \in E(G) \mid d_u + d_v = i\} \\ &\qquad\qquad \forall i : 2\delta \le i \le 2\Delta, \\ E_j^{*} &= \{uv \in E(G) \mid d_u \times d_v = j\} \quad \forall j : \delta^2 \le j \le \Delta^2. \end{aligned} \tag{16}$$

Proof of Theorem 2. Let PAH_k be the Polycyclic Aromatic Hydrocarbon for all integer numbers k. From the general representation of PAH_k in Figure 2, one can see that in this hydrocarbon molecular family there are $6k^2 + 6k$ vertices/atoms ($= |V(PAH_k)|$) such that $6k^2$ of them are carbon atoms and also $6k$ of them are hydrogen atoms. In other words,

$$\begin{aligned} V_3 &= V_C = \{v \in V(PAH_k) \mid d_v = 3\}, \\ V_1 &= V_H = \{v \in V(PAH_k) \mid d_v = 1\}. \end{aligned} \tag{17}$$

Thus, there are $(3 \times 6k^2 + 1 \times 6k)/2 = 9k^2 + 3k$ edges/chemical bonds ($= |E(PAH_n)|$) in PAH_k.

Now, by using Definition 6 and according to Figure 2, one can see that in hydrocarbon molecules PAH_k all hydrogen atoms have one connection and the degree of them is $d_{\text{Hydrogen}} = 1$ and there are 3 edges/chemical bonds for all carbon atoms; thus, $d_{\text{Carbon}} = 3$.

Therefore, we have two partitions of the vertex set $V(PAH_n)$ of Polycyclic Aromatic.

Hydrocarbons PAH_k are as follows:

$$\begin{aligned} E_4 &= E_3^* \\ &= \{e = uv = HC \in E(\mathrm{PAH}_n) \mid d_H = 1,\ d_C = 3\}, \\ E_6 &= E_9^* \\ &= \{e = uv = CC \in E(\mathrm{PAH}_n) \mid d_C = d_C = 3\}. \end{aligned} \tag{18}$$

On the other hand, from Figure 2 and [45, 46], we can see that $|E_4| = |E_3^*| = 6k$ and $|E_6| = |E_9^*| = 9k^2 - 3k$.

Here, we have the following computations for the Hyper-Zagreb index of the Polycyclic Aromatic Hydrocarbons PAH_k $(\forall k \in \mathbb{N})$ as follows:

$$\begin{aligned} HM(\mathrm{PAH}_k) &= \sum_{e=uv\in E(\mathrm{PAH}_k)} (d_u + d_v)^2 \\ &= \sum_{uv\in E_4\subseteq E(\mathrm{PAH}_k)} (d_u + d_v)^2 \\ &\quad + \sum_{uv\in E_6\subseteq E(\mathrm{PAH}_k)} (d_u + d_v)^2 \\ &= \sum_{uv\in E_4\subseteq E(\mathrm{PAH}_k)} (d_C + d_H)^2 \\ &\quad + \sum_{uv\in E_6\subseteq E(\mathrm{PAH}_k)} (d_C + d_C)^2 \\ &= 16\times|E_4| + 36\times|E_6| \\ &= 16\times(6k) + 36\times\left(9k^2 - 3k\right) \\ &= 12k(27k - 1). \end{aligned} \tag{19}$$

Here, we complete the proof of Theorem 2. □

Proof of Theorem 4. Consider the Polycyclic Aromatic Hydrocarbons PAH_k with $6k^2+6k$ vertices/atoms and $9k^2+3k$ edges. Then, by using the results from the above proof, we have the following computations for the general Randić and sum-connectivity indices of PAH_k $(\forall k \in \mathbb{N},\ \forall \alpha \in \mathbb{Q})$:

$$\begin{aligned} R^\alpha(\mathrm{PAH}_k) &= \sum_{e=uv\in E(\mathrm{PAH}_k)} (d_u d_v)^\alpha \\ &= \sum_{HC\in E_3^*} (d_H d_C)^\alpha + \sum_{CC\in E_9^*} (d_C d_C)^\alpha \\ &= |E_3^*|\times(3)^\alpha + |E_9^*|\times(9)^\alpha \\ &= 3^\alpha(6k) + 3^{2\alpha}\left(9k^2 - 3k\right) \\ &= 3k\left(3^{2\alpha+1}k + 3^\alpha\left(2 - 3^\alpha\right)\right), \\ X^\alpha(\mathrm{PAH}_k) &= \sum_{e=uv\in E(\mathrm{PAH}_k)} (d_u + d_v)^\alpha \\ &= \sum_{HC\in E_4} (d_H + d_C)^\alpha + \sum_{CC\in E_6} (d_C + d_C)^\alpha \\ &= |E_4|\times(4)^\alpha + |E_6|\times(6)^\alpha \\ &= 2^{2\alpha}(6k) + 6^\alpha\left(9k^2 - 3k\right) \\ &= 2^\alpha 3k\left(3^{\alpha+1}k - 3^\alpha + 2^{\alpha+1}\right). \end{aligned} \tag{20}$$

□

Proof of Theorem 5. Let PAH_k be the Polycyclic Aromatic Hydrocarbon for all integer numbers k. By results from proof of Theorem 2, we see that the Harmonic index and Harmonic polynomial of PAH_k $(\forall k \in \mathbb{N})$ are equal to

$$\begin{aligned} H(\mathrm{PAH}_k) &= \sum_{uv\in E(\mathrm{PAH}_k)} \frac{2}{d_u + d_v} \\ &= \sum_{uv\in E(\mathrm{PAH}_k)} \frac{2}{d_u + d_v} \\ &\quad + \sum_{uv\in E(\mathrm{PAH}_k)} \frac{2}{d_u + d_v} \\ &= \sum_{uv\in E_4} \frac{2}{d_H + d_C} + \sum_{uv\in E_6} \frac{2}{d_C + d_C} \\ &= \frac{2}{4}|E_4| + \frac{2}{6}|E_6| \\ &= \frac{2}{4}(6k) + \frac{2}{6}\left(9k^2 - 3k\right) \\ &= 3k + \left(3k^2 - k\right) = 3k^2 + 2k, \\ H(\mathrm{PAH}_k, x) &= \sum_{uv\in E(\mathrm{PAH}_k)} 2x^{(d_v+d_v-1)} \\ &= \sum_{HC\in E_4} 2x^{(d_H+d_C-1)} \\ &\quad + \sum_{CC\in E_6} 2x^{(d_C+d_C-1)} \\ &= 2|E_4|x^3 + 2|E_6|x^5 \\ &= 12kx^3 + 6k(3k-1)x^5. \end{aligned} \tag{21}$$

Here, the proof of Theorem 5 was completed. □

Competing Interests

The authors declare that there is no conflict of interests regarding the publication of this paper.

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