Some Connectivity Indices of Polycyclic Aromatic Hydrocarbons (PAHs)

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ABSTRACT

Let \( G=(V, E) \) be a molecular graph, such that in the simple connected graph \( G \), vertices represent atoms and edges represent bonds. A connectivity index is a real number related to the structure of connected graph \( G \) and is invariant under graph automorphism. There exits many structure in graph theory, with applied in chemical and nano science and vice versa.

In this paper, we focus on the structure of Polycyclic Aromatic Hydrocarbons (PAHs) and computing some connectivity indices of this family of hydrocarbon structures.

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1. Introduction

Let \( G=(V, E) \) be a simple finite molecular graph with the vertex set \( V(G) \) and the edge set \( E(G) \), \( |V(G)|=n, |E(G)|=e \) are the number of vertices and edges. In chemical graph theory, the vertices correspond to the atoms and the edges correspond to the bonds and the number of adjacent of vertex \( v \) is its degree, which denoted by \( d_v \). The vertices \( u \) and \( v \) are adjacent if there exist an edge \( e=uv \) between them.

In graph theory, we have many different topological indices of an arbitrary graph \( G \). A topological index of a graph is a real number related to the structure of graph which is invariant under graph automorphism. In particular, if \( G \) is the connected graph, we say connectivity topological index (for simply connectivity index). A connected graph is a graph such that there exists a path between all pairs of vertices. Some simplest topological indices are \( n, e, d \), and \( d(u,v) \). The distance \( d(u,v) \) between two vertices \( u \) and \( v \) is the length of the shortest path between \( u \) and \( v \) in the graph. Therefore, the number of edges \( e \) is the number of vertex pairs at unit.

In 1975 M. Randić proposed a structural descriptor called the branching index [1-2] that later became the well-known Randić molecular connectivity index (or simply Randić index). Motivated by the definition of Randić connectivity index based on the end-vertices degrees of edges in a graph and its formula is equal to:

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

Recently, a closely related variant of Randić connectivity index called the sum-connectivity index was introduced by Zhou and Trinajstić [3-4] in 2008. Sum-connectivity index \( X(G) \) is defined as

\[
X(G) = \sum_{u,v \in V(G)} \frac{1}{\sqrt{d_u + d_v}}
\]

where \( d_u \) and \( d_v \) are the degrees of the vertices \( u \) and \( v \), respectively.

In 2009, Vukičević and Furtula [5] proposed two topological indices named geometric-arithmetic index and atom-bond connectivity index (we denote by \( GA(G) \) and \( ABC(G) \), respectively.). They are defined as follows:

\[
GA(G) = \sum_{e=uv \in E(G)} 2\sqrt{d_u d_v}
\]

\[
ABC(G) = \sum_{e=uv \in E(G)} \sqrt{d_u + d_v - 2}
\]

In chemical graph theory, these connectivity indices are very important and have very chemical applications, mathematical properties. Some basic properties of these indices can be found in the recent letters. For more study, see reference [8-19].
addition, we need to compute these connectivity indices of a molecular graph \( G \).

**Definition 1.** [12] Let \( G \) be the molecular graph and \( d_v \) is degree of vertex \( v \in V(G) \). We divide vertex set \( V(G) \) and edge set \( E(G) \) of graph \( G \) to several partitions, as follow:

\[
\forall i, \delta \in \mathbb{A}; \quad V_i = \{v \in V(G) \mid d_v = i\},
\]

\[
\forall j, 2\delta \in \mathbb{A}; \quad E_j = \{e = uv \in E(G) \mid d_v + d_u = j\}
\]

And

\[
\forall k, \delta \in \mathbb{A}; \quad E_k^* = \{e = uv \in E(G) \mid d_v \times d_u = k\}
\]

Notice that \( \delta = \min\{d_v \mid v \in V(G)\} \) and

\[\Delta = \max\{d_v \mid v \in V(G)\}\] where these three first members and the general representation of this hydrocarbons (we denote \( PAH_n \)) are shown in Figure 1 and Figure 2.

**2. Main results and discussion**

In this section, we compute Randić connectivity index, sum-connectivity index, geometric-arithmetic index and atom-bond connectivity index of a family of hydrocarbon molecules, which called **Polycyclic Aromatic Hydrocarbons (PAHs)**. Large polycyclic aromatic hydrocarbons (PAHs) are ubiquitous combustion products. They have been implicated as carcinogens and play a role in graphitisation of organic materials [20]. In addition, they are of interest as molecular analogues of graphite [21] as candidates for interstellar species [22] and as buildingblocks of functional materials for device applications [21-23]. Synthetic routes to PAHs are available [24] and a detailed knowledge of all these features would therefore be necessary for the tuning of molecular properties towards specific applications (see the references [20-28]).

The PAHs can be thought 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 [29-31] and references therein.

This polycyclic aromatic hydrocarbons (or PAH family) are very similar properties to one of famous family of Benzenoid system (**Circumcoronene Homologous Series of Benzenoid**). The properties and applications of Benzenoid system are presented in many papers, reader can see the paper series [31-55] and references therein.

Herein this paper, we denote the first members of this hydrocarbon family as follow:

- **PAH_1** be the **Benzene** with six carbon (C) and six hydrogen (H) atoms,
- **PAH_2** be the **Coronene** with 24 carbon and twelve hydrogen atoms,
- **PAH_3** be the **Circumcoronene** with 54 carbon and eighteen hydrogen atoms.

From above figure, one can see that the polycyclic aromatic hydrocarbon \( PAH_n \) has \( 6n^2 \) carbon (C) and \( 6n \) hydrogen (H) atoms.

Now, by these terminologies, we have following theorems.

**Theorem 1.** Consider the polycyclic aromatic hydrocarbons molecules \( PAH_n (n \in \mathbb{N}) \), then

The Randić connectivity index is equal to:

\[\chi(\text{PAH}_n) = 3n^2 + (2\sqrt{3} - 1)n\]

The Sum-connectivity index of \( PAH_n \) is equal to:

\[X(\text{PAH}_n) = \left(\frac{3\sqrt{6}}{2}\right)n^2 + \left(\frac{6 - \sqrt{6}}{2}\right)n\]

**Proof.** Let \( PAH_n (n \in \mathbb{N}) \), be the general representation of this polycyclic aromatic hydrocarbon. This molecular graph has \( 6n^2+6n \) vertices/atoms (=\( |V(PAH_n)| \)) such that \( 6n^2 \) of them are carbon atoms and also \( 6n \) of them hydrogen atoms. Thus, the number of edge in this hydrocarbon molecule (chemical bonds) is equal to:

\[|E(PAH_n)| = \frac{3 \times 6n^2 + 1 \times 6n}{2} = 9n^2 + 3n\]

According to Definition 1, it is easy to see that in a hydrocarbon molecules all hydrogen atoms have one connection and in other words mathematical graph degree of hydrogen atoms is \( d_{\text{hydrogen}}=1 \) and whereas for a carbon atom may be \( d_{\text{carbon}}=4 \) (especially **Graphite** and **Diamond** molecules), 3, 2 or 1 (In especial molecule \( C_2 \)).
From Figure 2, one can to see that all carbon atoms of \( \text{PAH}_n \) have degree three \( d_{\text{carbon}}=3 \) (or simply \( d_C \)) and obviously the edge/bond set of polycyclic aromatic hydrocarbon can be dividing to two partitions, e.g. \( E_4 \) (or \( E^*_4 \)) and \( E_6 \) (or \( E^*_6 \)). On other hands,

\[
E_4 = E^*_4 = \{e = HC \in E(\text{PAH}_n) \mid d_H + d_C = 4\}
\]
and \( |E_4| = 6n \)

Also, \( E_6 = E^*_6 = \{e = CC \in E(\text{PAH}_n) \mid d_C + d_C = 6\} \)
and \( |E_6| = 9n^2 \cdot 3n \)

From Figure 2 and by usage of the definitions of connectivity indices, we can compute Randić connectivity index and Sum-connectivity index of polycyclic aromatic hydrocarbon \( \text{PAH}_n \) as follows:

\[
\chi(\text{PAH}_n) = \sum_{HC \in E_4} \frac{1}{\sqrt{d_H \cdot d_C}} + \sum_{CC \in E_6} \frac{1}{\sqrt{d_C \cdot d_C}}
\]

\[
= |E^*_4| + |E^*_6| \cdot \sqrt{\frac{3}{5}}
\]

\[
= \sqrt{3}(9n^2 \cdot 3n) + \sqrt{\frac{3}{5}}(6n)
\]

\[
= 5n^3 + (2\sqrt{3} \cdot 1)n
\]

Also, the sum-connectivity index of \( \text{PAH}_n \) is

\[
X(\text{PAH}_n) = \sum_{HC \in E_4} \frac{1}{\sqrt{d_H + d_C}} + \sum_{CC \in E_6} \frac{1}{\sqrt{d_C + d_C}}
\]

\[
= \frac{|E^*_4|}{\sqrt{4}} + \frac{|E^*_6|}{\sqrt{6}}
\]

\[
= \frac{\sqrt{6}(6n)}{6} + \frac{\sqrt{3}}{6}(9n^2 \cdot 3n)
\]

\[
= \frac{3\sqrt{6}}{2}n^3 + \left(6 - \frac{\sqrt{6}}{2}\right)n
\]

\[\textbf{Theorem 2.} \text{For all } n \in \mathbb{Z}^+, \text{the Geometric-Arithmetic index and Atom-Bond connectivity index of polycyclic aromatic hydrocarbons molecules } \text{PAH}_n \text{ are equal to}
\]

\[
\text{GA}(\text{PAH}_n) = 9n^2 + 3(\sqrt{3} - 1)n
\]

\[
\text{ABC}(\text{PAH}_n) = 6n^2 + 2(\sqrt{6} - 1)n
\]

\[\textbf{Proof.} \text{By use of results from above proof, the proof is clear and we have following computations for two connectivity topological indices “geometric-arithmetic” and “atom-bond connectivity” of } \text{PAH}_n \text{ as follows:}
\]

\[
\text{GA}(\text{PAH}_n) = \sum_{uv \in E(\text{PAH}_n)} 2\sqrt{d_u d_v}
\]

\[
= \sum_{HC \in E_4} 2\sqrt{d_H d_C} + \sum_{CC \in E_6} 2\sqrt{d_C d_C}
\]

\[
= \frac{2\sqrt{3}}{4} + \sum_{E_4} 2\sqrt{3}
\]

\[
= \frac{3\sqrt{6}}{2}n^3 + \left(6 - \frac{\sqrt{6}}{2}\right)n
\]

\[
= 5n^3 + (2\sqrt{3} \cdot 1)n
\]

\[
\text{ABC}(\text{PAH}_n) = \sum_{uv \in E(\text{PAH}_n)} \sqrt{d_u + d_v - 2}
\]

\[
= \sum_{HC \in E_4} \sqrt{d_H + d_C - 2} + \sum_{CC \in E_6} \sqrt{d_C + d_C - 2}
\]

\[
= \frac{\sqrt{6}}{3}(6n) + \frac{\sqrt{3}}{6}(9n^2 \cdot 3n)
\]

\[
= 6n^2 + 2(\sqrt{6} - 1)n
\]

Here, we complete the proof of Theorem 2. \( \blacksquare \)

\[\textbf{3. Conclusion:}
\]

In chemical graph theory, there exits many structure. These structures have very application in chemical and nano science. And vice versa the chemical compounds and nano structures have many mathematics properties in mathematics graph theory. In this paper, we focus on the structure of a family of hydrocarbon molecules, which called polycyclic aromatic hydrocarbons (PAHs). And formulas of some connectivity topological indices of this family of hydrocarbon structures are determined for the first time.
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