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Research Article

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Computing the fourth atom-bond connectivity index of the Polycyclic Aromatic Hydrocarbons

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Abstract Among topological descriptors topological indices are very important and they have a prominent role in chemistry. One of them is atom-bond connectivity (*ABC*) index defined as $ABC(G)=\sum_{uv\in E(G)}\sqrt{\frac{d_u+d_v-2}{d_ud_v}}$, where d_v is the degree of vertex *v*. Recently, a new version of atom-bond connectivity (ABC_4) index was introduced by *M. Ghorbani et. al.* [38] in 2010 and is defined as $ABC_4(G)=\sum_{uv\in E(G)}\sqrt{\frac{S_u+S_v-2}{S_uS_v}}$, where $S_u=\sum_{v\in N_G(u)}d_v$ and $N_G(u)$ = $\{v\in V(G)|uvE(G)\}$. In this paper we compute this new topological index for Polycyclic Aromatic Hydrocarbons PAH_k.

Keywords Topological index, Atom bond connectivity index. Polycyclic Aromatic Hydrocarbons PAH_k.

Introduction

Let $G=(V;E)$ be a simple molecular graph without direction, multiple edges and loops, the vertex and edge sets of it are represented by $V=V(G)$ and $E=E(G)$, respectively. In chemical graphs, the vertices correspond to the atoms of the molecule, and the edges represent to the chemical bonds. Also, if *e* is an edge of *G*, connecting the vertices *u* and *v*, then we write $e=uv$ and say "*u* and *v* are adjacent".

Mathematical chemistry is a branch of theoretical chemistry for discussion and prediction of the molecular structure using mathematical methods without necessarily referring to quantum mechanics. Chemical graph theory is a branch of mathematical chemistry which applies graph theory to mathematical modeling of chemical phenomena [1-3]. This theory had an important effect on the development of the chemical sciences.

In mathematical chemistry, numbers encoding certain structural features of organic molecules and derived from the corresponding molecular graph, are called *graph invariants* or more commonly *topological indices*.

Among topological descriptors, connectivity indices are very important and they have a prominent role in chemistry. In other words, if *G* be the connected graph, then we can introduce many connectivity topological indexes for it, by distinct and different definition. A connected graph is a graph such that there is a path between all pairs of vertices.

One of the best known and widely used is the connectivity index, introduced in 1975 by *Milan Randić* [4], who has shown this index to reflect molecular branching and defined as follows:

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

where d_u denotes G degree of vertex u.

In 2009, *Furtula* [5] proposed the first atom-bond connectivity index of a graph G as:

$$ABC_1(G)=\sum_{uv\in E(G)}\sqrt{\frac{d_u+d_v-2}{d_u d_v}}$$

The second atom-bond connectivity index is introduced by *A. Graovac* [6]. It is defined as follows

$$ABC_2=\sum_{uv\in E(G)}\sqrt{\frac{n_u+n_v-2}{n_u n_v}}$$

where n_v is the number of vertices of graph G whose distance to the vertex v is smaller than the distance to the vertex u.

Farahani [7] proposed the third atom-bond connectivity index of G as follows:

$$ABC_3(G)=\sum_{e=uv\in E(G)}\sqrt{\frac{m_v+m_u-2}{m_v.m_u}}$$

Recently, *Ghorbani* [8] defined a new version of atom-bond connectivity index. It is named as *Fourth atom-bond connectivity index* and defined as

$$ABC_4=\sum_{uv\in E(G)}\sqrt{\frac{S_u+S_v-2}{S_u S_v}}$$

where S_u is the sum of degrees of all neighbor of vertex u in graph G. Reader can found the history and results on this family of indices in [9-12].

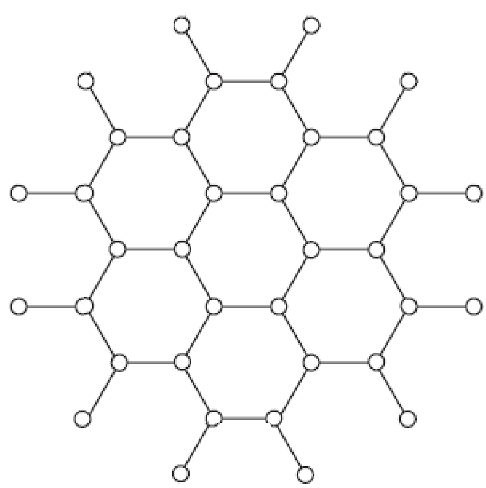

Figure 1: Polycyclic Aromatic Hydrocarbon PAH_k for k=2.

Results

In this section, we computed the fourth version of atom-bond connectivity index of *Polycyclic Aromatic Hydrocarbons* PAH_k. A 2-dimensional lattice of Polycyclic Aromatic Hydrocarbon PAH_k is shown in Figure 2. It has $6k^2+6k$ vertices and $9k^2+3k$ edges.

Polycyclic Aromatic Hydrocarbons (PAH_k) are a group of more than 100 different chemicals that are formed during the incomplete burning of garbage, gas, oil, coal or other organic materials. Some PAH_k are manufactured. These PAH_k usually exist as colorless, white, pale yellow-green solids. The PAH_k discussed in this paper is a family of hydrocarbons containing several copies of benzene on circumference. A member of this family for $k=2$ is shown in Figure 1 and a general representation is shown in Figure 2.

In [13-35] some topological indices of molecular graphs *Polycyclic Aromatic Hydrocarbons* PAH_k are computed. In this paper, we continue this work to compute the fourth atom-bond connectivity index of *Polycyclic Aromatic Hydrocarbons* PAH_k. Our notation is standard and mainly taken from [36-37].

Theorem 1: Consider the graph of *Polycyclic Aromatic Hydrocarbon* PAH_k, then the fourth atomic connectivity index of PAH_k is equal to

$$ABC_4(PAH_k) = 4k^2 + k\left(6\sqrt{\frac{8}{21}} + 4\sqrt{2} - \frac{20}{3}\right) + \left(\frac{6\sqrt{12}}{7} - 4\sqrt{2} + \frac{8}{3}\right)$$

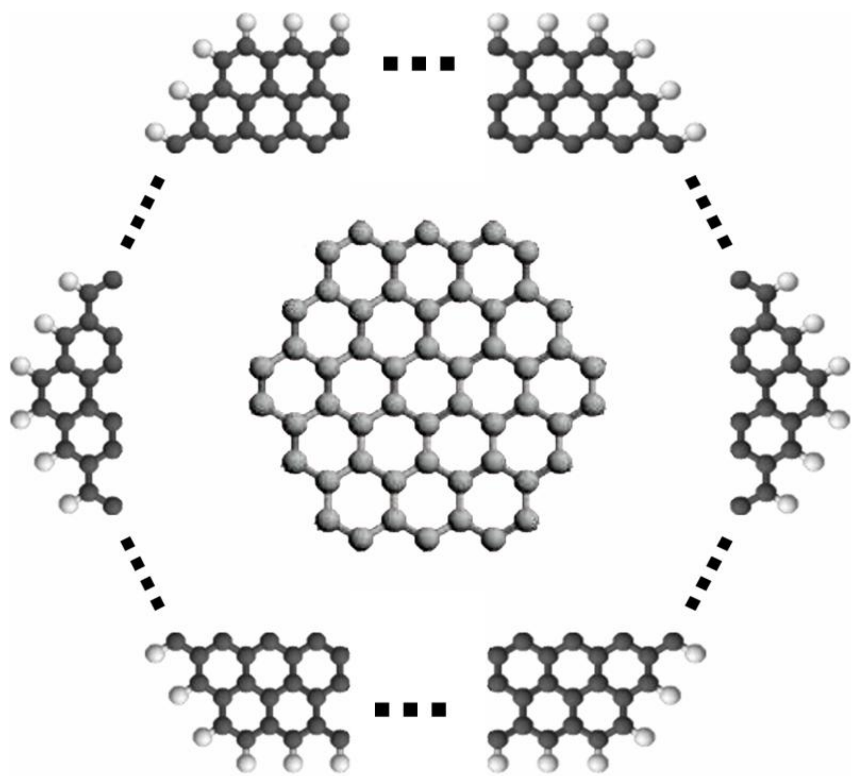

Figure 2: 2-dimensional representation of Polycyclic Aromatic Hydrocarbon PAH_k.

Proof: From Figure 2, we noticed that in the structure of PAH_k vertices have degrees 1 or 3. We denote the sets of vertices with degree 1 and degree 3 as $V_1=\{v\in V(G)\,|\,d_v=1\}$ and $V_3=\{v\in V(G)\,|\,d_v=3\}$. From V_1 and V_2, we have edge partitions $E_4=\{uv\in E(PAH_k)\,|\,d_u+d_v=4\}$ and $E_6=\{uv\in E(PAH_k)\,|\,d_u+d_v=6\}$ and $|E_4|=6k$, $|E_6|=9k^2-3k$. Clearly, the sum of degrees of vertices for each edge of PAH_k is as follows:

- There are $6k$ edges $e=uv$ for which, $S_u=3$, $S_v=7$ when $u \in V_1$, $v \in V_3$ and $uv \in E_4$
- There are 6 edges $e=uv$ for which, $S_u=S_v=7$ when $u,v \in V_6$ and $uv \in E_6$
- There are $12(k-1)$ edges $e=uv$ for which, $S_u=7$, $S_v=9$ when $u,v \in V_6$ and $uv \in E_6$
- There are $9k^2-15k+6$ edges $e=uv$ for which, $S_u=S_v=9$ when $u,v \in V_3$ and $uv \in E_6$.

From the above calculation, now we can obtain the required result.

$$ABC_4(PAH_k)= \sum_{uv \in E(G)} \sqrt{\frac{S_u+S_v-2}{S_uS_v}}$$

$$=6k\sqrt{\frac{3+7-2}{3\times 7}}+6\sqrt{\frac{7+7-2}{7\times 7}}+12(k-1)\sqrt{\frac{7+9-2}{7\times 9}}+(9k^2-15k+6)\sqrt{\frac{9+9-2}{9\times 9}}$$

$$=6k\sqrt{\frac{8}{21}}+\frac{6\sqrt{12}}{7}+4(k-1)\sqrt{2}+(9k^2-15k+6)\frac{4}{9}$$

$$=4k^2+k\left(6\sqrt{\frac{8}{21}}+4\sqrt{2}-\frac{20}{3}\right)+\left(\frac{6\sqrt{12}}{7}-4\sqrt{2}+\frac{8}{3}\right)$$

So, the proof is complete.

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