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Computing Atom-Bond Connectivity (ABC_4) index for Circumcoronene Series of Benzenoid

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ABSTRACT

Let *G=(V; E)* be a simple connected graph. The sets of vertices and edges of G are denoted by *V=V(G)* and *E=E (G),* respectively. In such a simple molecular graph, vertices represent atoms and edges represent bonds. The Atom-Bond Connectivity (*ABC*) index is a topological index was defined as $ABC(G)=\sum_{uv\in E(G)}\sqrt{\frac{d_u+d_v-2}{d_u d_v}}$, where d_v denotes degree of vertex *v*. In 2010, a new version of Atom-Bond Connectivity (*ABC*$_4$) index was defined by *M. Ghorbani et. al* as $ABC_4(G)=\sum_{uv\in E(G)}\sqrt{\frac{S_u+S_v-2}{S_u S_v}}$, where $S_u=\sum_{v\in N_G(u)}d_v$ and $N_G(u)=\{v\in V(G)|uvE(G)\}$. The goal of this paper is to compute the *ABC*4 index for Circumcoronene Series of Benzenoid

Indexing terms/Keywords

Atom-Bond Connectivity (*ABC*$_4$) index, Molecular Graph, Circumcoronene Series of Benzenoid.

SUBJECT CLASSIFICATION

E.g., Mathematics Subject Classification; 05C05, 05C12

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INTRODUCTION

Let *G=(V;E)* be a simple molecular graph without directed and multiple edges and without 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. Note that hydrogen atoms are often omitted. 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". A connected graph is a graph such that there is a path between all pairs of vertices.

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. 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.

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

where d_u denotes *G* degree of vertex *u*.

One of the important classes of connectivity indices is atom-bond connectivity (ABC) index defined as [5]

$$ABC_{\text{general}}(G) = \sum_{uv \in E(G)} \sqrt{\frac{Q_u + Q_v - 2}{Q_u Q_v}},$$

where Q_v is some quantity that in a unique manner can be associated with the vertex *v* of the graph *G*.

In 2009, *Furtula et al.* [6] introduced the first member of this class (atom-bond connectivity (*ABC*) index), by setting Q_v to be the degree of a vertex *v* d_v, which it has been applied up until now to study the stability of alkanes and the strain energy of cycloalkanes. This index is defined as follows:

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

The second member of this class was considered by *A. Graovac* and *M. Ghorbani* [7], by setting Q_u to be n_u as follows*:*

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

where n_u denotes the number of vertices of *G* whose distances to vertex *u* are smaller than those to other vertex *v* of the edge *e=uv* $(n_u = \{x \mid x \in V(G), d(u,x) < d(x,v)\})$ and n_v is defined analogously.

The third members of this class was introduced by *M.R. Farahani* [8, 9], as follow:

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

where m_u denotes the number of vertices of *G* whose distances to vertex *u* are smaller than those to other vertex *v* of the edge *e=uv* $(m_u = \{f \mid f \in E(G), d(u,f) < d(f,v)\})$ and m_v is defined analogously.

In 2010, a new version of Atom-Bond Connectivity (ABC_4) index was defined by *M. Ghorbani et. al* [10] as

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

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where S_v is the summation of degrees of all neighbors of vertex v in G. In other words, $S_u = \sum_{v \in N_G(u)} d_v$ and $N_G(u)=\{v \in V(G) | uv E(G)\}$.

The goal of this paper is to compute the fourth atom-bond connectivity index ABC_4 index for Circumcoronene Series of Benzenoid. Here our notation is standard and mainly taken from standard books of chemical graph theory [1-3].

Main Results and Discussions

The goal of this section is to computing the ABC_4 index for Circumcoronene Series of Benzenoid. The circumcoronene homologous series of benzenoid is family of molecular graph, which consist several copy of benzene C_6 on circumference. The first terms of this series are H_1=benzene, H_2=coronene, H_3=circumcoronene, H_4=circumcircumcoronene, see Figure 1, where they are shown, also for more study and historical details of this benzenoid molecular graphs see the paper series [11-29].

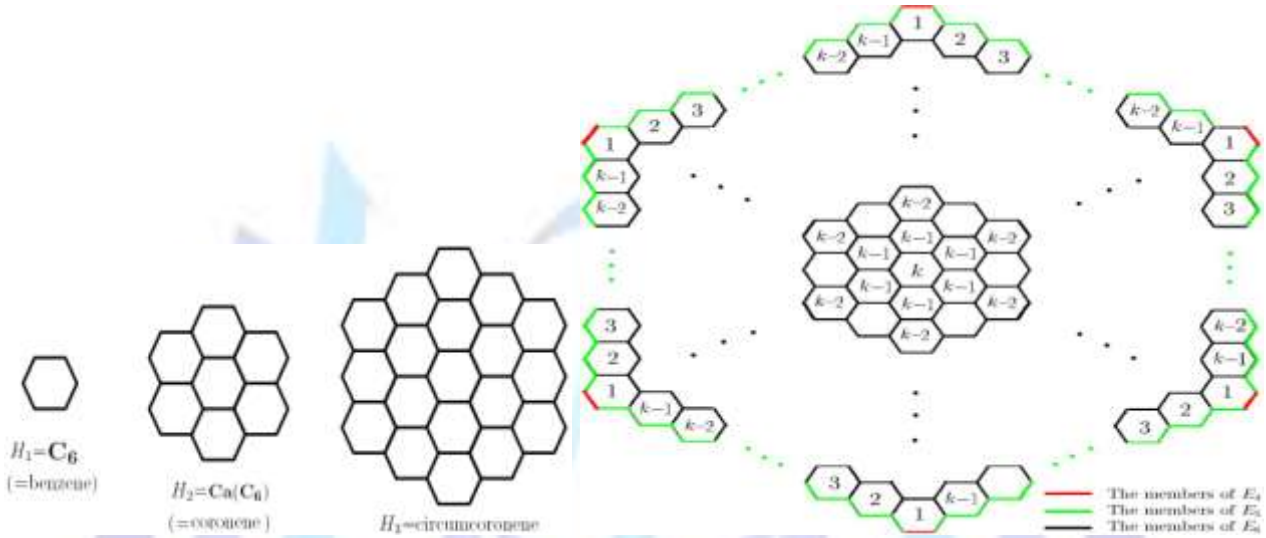

Fig 1. The first three graphs H_1, H_2, H_3 and general representation H_k of the circumcoronene series of benzenoid [16].

At frist, Consider the circumcoronene series of benzenoid H_k for all integer number $k \geq 1$ (Figure 1). From the structure of H_k (Figure 1), one can see that the number of vertices/atoms in this benzenoid molecular graph is equal to $|V(H_k)|=6k^2$ and the number of edges/bonds is equal to $|E(H_k)|= \frac{3\times 6k\ \ k-1\ +2\times 6k}{2} = 9k^2-3k$. Because, the number of vertices/atoms as degrees 2 and 3 are equal to $6k$ and $6k(k-1)$ and in circumcoronene series of benzenoid molecule, there are two partitions $V_2 = \{v \in V(G) | d_v = 2\}$ and $V_3 = \{v \in V(G) | d_v = 3\}$ of vertices. These partitions imply that there are three partitions E_4, E_5 and E_6 of edges set of molecule H_k with size 6, $12(k-1)$ and $9k^2-15k+6$, respectively. Clearly, we mark the members of E_4, E_5 and E_6 by red, green and black color in Figure1.

From Figure 1, one can see that the summation of degrees of vertices of molecule benzenoid H_k are in four types, as follow:

- $S_v = S_u = 2+3 = 5$ for $u,v \in V_2$ and $uv \in E_4$
- $S_u = d_v + d_v = 6$ for $u \in V_2$, $v \in V_3$ and $uv \in E_5$
- $S_u = d_v + d_v + 3 = 7$ for $u \in V_3$, $v \in V_2$ and $uv \in E_5$
- $S_u = S_v = d_v + d_u + 3 = 9$ for $u,v \in V_3$ and $uv \in E_6$

So, the fourth atom-bond connectivity index for circumcoronene series of benzenoid H_k ($\forall$ $k \geq 1$) will be

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

$$= 6\sqrt{\frac{5+5-2}{5\times 5}} + 6\sqrt{\frac{5+7-2}{5\times 7}} + 2\times 6\ \ k-2\ \sqrt{\frac{6+7-2}{6\times 7}} + 6\ \ k-1\ \sqrt{\frac{7+9-2}{7\times 9}} + |E\ \ H_{k-1}\ |\sqrt{\frac{9+9-2}{9\times 9}}$$

$$= \frac{12\sqrt{2}}{5} + \sqrt{30} + 2\sqrt{\frac{66}{7}}\ \ k-2\ \ + 2\sqrt{2}\ \ k-1\ \ + \frac{4}{3}(3k^2-7k+4)$$

$$= 4k^2 + 2\left(\sqrt{\frac{66}{7}} + \sqrt{2} - 14\right)k + \left(\frac{2\sqrt{2}}{5} + \sqrt{30} + 16 - 4\sqrt{\frac{66}{7}}\right)$$

Finally, fourth atom-bond connectivity index for circumcoronene series of benzenoid H_k is

$$ABC_4(H_k) = 4k^2 - 19.03038k + 9.76052.$$

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