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

\[
ABC(G) = \sum_{uv \in E(G)} \frac{d_u + d_v - 2}{d_ud_v},
\]

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

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

where \(S_u = \sum_{v \in N_G(u)} d_v\) and \(N_G(u) = \{v \in V(G) \mid uv \in E(G)\}\). 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
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.

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

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]

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

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 $Q_v$ to be $n_v$ as follows:

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

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

In 2010, a new version of Atom-Bond Connectivity (ABC4) index was defined by M. Ghorbani et. al [10] as

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

where $s_u$ denotes the number of vertices of $G$ whose distances to vertex $u$ are smaller than those to other vertex $v$ of the edge $e=uv$ ($s_u = \{f \mid f \in E(G), d(u,f) < d(f,v)\}$) and $s_u$ is defined analogously.
where \( S_v \) is the summation of degrees of all neighbors of vertex \( v \) in \( G \). In other words, \( S_v = \sum_{u \in N_G(v)} d_u \) and \( N_G(u) = \{v \in V(G) \mid uv \in E(G)\} \).

The goal of this paper is to compute the fourth atom-bond connectivity index \( ABC_4 \) 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 \( H_1=\text{benzene}, H_2=\text{coronene}, H_3=\text{circumcoronene}, H_4=\text{circumcircumcoronene} \), 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].](image)

At first, 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 \( |E(H_k)|= \frac{3 \times 6k^2}{2} - \frac{3k^2}{2} \). 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 \( V_2 = \{v \in V(G) \mid d_v = 2\} \) and \( V_3 = \{v \in V(G) \mid d_v = 3\} \) 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 Figure 1.

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

- \( S_u = S_v = 2+3 = 5 \) 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 \( uv \in E_5 \)
- \( S_u = S_v = d_v + d_v + 3 = 9 \) 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

\[
ABC_4(H_k) = \sum_{u,v \in E(G)} \frac{S_u + S_v - 2}{S_u S_v} = 6 \cdot \frac{S_2(S_2)}{5 \times 5} + 6 \cdot \frac{S_2(S_2)}{5 \times 7} + 6 \cdot \frac{S_2(S_2)}{6 \times 6} + 6 \cdot \frac{S_2(S_2)}{7 \times 9} + |E_4 : H_{k-1}| \cdot \frac{9 + 9 - 2}{9 \times 9} + 2 \cdot \sqrt{6} \cdot \sqrt{6} \cdot \frac{3k^2-15k+6}{3k^2-15k+6} + 4 \cdot \frac{3k^2-7k+4}{3k^2-7k+4}
\]

\[
= \frac{12 \sqrt{3}}{5} + \sqrt{30} + 2 \sqrt{6} \cdot \sqrt{6} \cdot \frac{3k^2-15k+6}{3k^2-15k+6} + 4 \cdot \frac{3k^2-7k+4}{3k^2-7k+4}
\]
Finally, fourth atom-bond connectivity index for circumcoronene series of benzenoid $H_k$ is

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

REFERENCES


