Atom Bond Connectivity Index of Carbon Nanocones and An Algorithm

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Abstract Let G be a chemical graph, where V(G) and E(G) are represented set of vertices and edges respectively. Atom bond connectivity index ABC(G) is related to degree of vertices of graph G. In this paper, we calculate the index for generalized carbon nanocones. Subsequently, an useful algorithm (pseudocode) are given. The goal of this paper is to further the study of ABC(G) index for generalized carbon nanocones.

Keywords: carbon nanocones, atom bond connectivity index, generalized formula, algorithm


1. Introduction

The graph theory has wide range of applied field and which is specially nanostructures of nanotechnology. Carbon nanotubes (CNT) were discovered by Sumio Iijima in 1991 [6]. Subsequently, carbon nanocones (CNC) were discovered by Ge and Sattler in 1994 [7] (See Figure 1). Recently, nanostructures involving carbon have been the focus of an intense research activity, which is driven to a large extent by the quest for new materials with miscellaneous applications.

A topological index of a chemical graph G is numeric quantity attributed to G. The topological indices are graph invariants and are used for quantitative structure-activity relationship (QSAR) and quantitative structure-property relationship (QSPR) [8,9]. The oldest topological index is Wiener index, which was presented by the chemist Harold Wiener in 1947 [10]. It is based on distance \(d(u,v)\) between any \(u\) and \(v\) atoms in chemical graph \(G\) and defined as follows:

\[
W(G) = \sum_{\{u,v\} \in V(G)} d(u,v).
\]

Now, we give some definitions. Let \(G\) be a basic chemical graph, in which edge sets are represented by \(E(G)\) and degree of vertex \(u\) is represented by \(d(u)\). In chemical graphs, the vertices of the graph attributed to the atoms of the molecule and the edges represent the chemical bonds. Atom bond connectivity index [2] defined as follows:

\[
ABC(G) = \sum_{u,v \in E(G)} \sqrt{\frac{d(u)+d(v)-2}{d(u)d(v)}}.
\]

In the research paper [11], the authors evaluated \(GA\) and \(ABC\) topological index of trigonal and tetragonal carbon nanocones.

In this paper, we aimed to develop atom bond connectivity index for generalized carbon nanocones.

![Figure 1](image_url) (a), (b) The one-pentagonal carbon nanocone (top and side view) (color figure available online)

2. Main Results

Let \(CNC_m[n] = C_m[n]\) be. Our notation is standard and mainly taken from standard book of graph theory such as [3,4,5]. Now we give to require theorems.
Theorem 1 [1]. Consider the graph of carbon nanocones $C_4[n]$. Then we have:

$$ABC(C_4[n]) = (n+1)(4n+2\sqrt{2}).$$

Theorem 2 [1]. Consider the graph of carbon nanocones $C_3[n]$. Then we have:

$$ABC(C_3[n]) = 5n^2 - 9n + 8 + \frac{(6n+3)\sqrt{2}}{2}.$$ 

Theorem 3. Consider the graph of pentagonal carbon nanocones $C_5[n]$. Then we have

$$ABC(C_5[n]) = \frac{15n^2 + 5n}{2} + \frac{(5+10n)\sqrt{2}}{2}. $$

Proof. Let us consider the graph $C_5[n]$ has $\left(\frac{15n^2 + 5n}{2}\right)$ edges and $5(n+1)^2$ vertices for all $n=1,2,3,\ldots$. On the other hand, there are $\left(\frac{15n^2 + 5n}{2}\right)$ edges of type $d(u)=d(v)=3$, 5 edges of type $d(u)=d(v)=2$ and $10n$ edges of type $d(u)=3$, $d(v)=2$. We get

$$ABC(C_5[n]) = \frac{15n^2 + 5n}{2} + \frac{(5+10n)\sqrt{2}}{2}. $$

Proposition 4. Consider the graph of pentagonal carbon nanocones $C_5[1]$. Then we have

$$ABC(C_5[1]) = \frac{20}{3} + \frac{15\sqrt{2}}{2}. $$

Proof. The graph of pentagonal carbon nanocones $C_5[1]$ is illustrated in Figure 2 and which has 25 edges. If $u$ and $v$ be endpoints on any edge then there exist, 10 edges of type $d(u)=d(v)=3$, 5 edges of type $d(u)=d(v)=2$, 10 edges of type $d(u)=3$, $d(v)=2$. This way,

$$ABC(C_5[1]) = 10 \times \frac{3+3-2}{9} + 5 \times \sqrt{\frac{2+2-2}{4}} + 10 \times \sqrt{\frac{3+3-2}{6}} = \frac{20}{3} + \frac{15\sqrt{2}}{2}. $$

Proposition 5. Consider the graph of pentagonal carbon nanocones $C_5[2]$. Then we have

$$ABC(C_5[2]) = \frac{70}{3} + \frac{25\sqrt{2}}{2}. $$

Proof. The graph of pentagonal carbon nanocones $C_5[2]$ is illustrated in Fig. 3 and which has 60 edges. 35 edges of type $d(u)=d(v)=3$, 5 edges of type $d(u)=d(v)=2$, 20 edges of type $d(u)=3$, $d(v)=2$. Then,

$$ABC(C_5[2]) = 35 \times \sqrt{\frac{3+3-2}{9}} + 5 \times \sqrt{\frac{2+2-2}{4}} + 20 \times \sqrt{\frac{3+3-2}{6}} = \frac{70}{3} + \frac{25\sqrt{2}}{2}. $$

Theorem 6. Consider the graph of heptagonal carbon nanocones $C_7[n]$. Then we have

$$ABC(C_7[n]) = \frac{7}{3}(3n^2 + n) + \frac{(7+14n)\sqrt{2}}{2}. $$

Proof. Let us consider the graph $C_7[n]$ has $\frac{7}{2}(3n^2 + 5n + 2)$ edges and $7(n+1)^2$ vertices for all $n=1,2,3,\ldots$. On the other hand, there are $\frac{7}{2}(3n^2 + n)$ edges of type $d(u)=d(v)=3$, 7 edges of type $d(u)=d(v)=2$ and $14n$ edges of type $d(u)=3$, $d(v)=2$. Hence,

$$ABC(C_7[n]) = \left(\frac{7}{2}(3n^2 + n)\right) + \frac{(7+14n)\sqrt{2}}{2}. $$

Proposition 7. Consider the graph of heptagonal carbon nanocones $C_7[1]$. Then we have

$$ABC(C_7[1]) = \frac{28}{3} + \frac{21\sqrt{2}}{2}. $$

Proof. The graph of heptagonal carbon nanocones $C_7[1]$ is illustrated in Figure 4 and which has 35 edges.
14 edges of type \( d(u) = d(v) = 3 \),
7 edges of type \( d(u) = d(v) = 2 \),
14 edges of type \( d(u) = 3, d(v) = 2 \), then we get,
\[
ABC(C_7[1]) = 14\times \sqrt{\frac{3+3-2}{9}} + 7\times \sqrt{\frac{2+2-2}{4}} + 14\times \sqrt{\frac{3+2-2}{6}} = \frac{28+21\sqrt{2}}{3}.
\]

**Proposition 8.** Consider the graph of heptagonal carbon nanocones \( C_7[2] \). Then we have
\[
C_7[2] = \frac{98}{3} + \frac{35\sqrt{2}}{2}.
\]
**Proof.** The graph of heptagonal carbon nanocones \( C_7[2] \) has 84 edges.
49 edges of type \( d(u) = d(v) = 3 \),
7 edges of type \( d(u) = d(v) = 2 \),
28 edges of type \( d(u) = 3, d(v) = 2 \), then we have
\[
ABC(C_7[2]) = 49\times \sqrt{\frac{3+3-2}{9}} + 7\times \sqrt{\frac{2+2-2}{4}} + 28\times \sqrt{\frac{3+2-2}{6}} = \frac{98+35\sqrt{2}}{3}.
\]
We conclude that the following theorem.
**Theorem 9.** Let \( m \geq 3 \) and \( n \geq 1 \) be positive integers. Then, we have the generalized formula
\[
ABC(C_m[n]) = \frac{m}{3}(3n^2+n)+\frac{m\sqrt{2}}{2}+mn\sqrt{2}.
\]
**Proof.** Let \( E_i, E_j \) and \( E_k \) (\( i, j \) and \( k \) are arbitrary positive integers) are subsets of \( E(C_m[n]) \). Then,
\[
E_i = \{uv \in E(G) | d(u) = d(v) = 3\}, |E_i| = m\left(3n^2+n\right)/2,
E_j = \{uv \in E(G) | d(u) = d(v) = 2\}, |E_j| = m,
E_k = \{uv \in E(G) | d(u) = 3, d(v) = 2\}, |E_k| = 2mn.
\]
Hence,
\[
ABC(C_m[n]) = \frac{m}{3}(3n^2+n)+\sqrt{\frac{3+3-2}{9}}+m\sqrt{\frac{2+2-2}{4}}+2mn\sqrt{2}.
\]
We get
\[
ABC(C_8[1]) = \frac{m}{3}(3n^2+n)+\frac{m\sqrt{2}}{2}+mn\sqrt{2}.
\]
The proof is completed.
In Table 1 and Table 2, the numbers of edges of type \( d(u)=d(v)=3 \), \( d(u)=d(v)=2 \) and \( d(u)=3, d(v)=2 \) have been shown as respectively. Also, the values of ABC index have been calculated for some \( C_5[n] \) and \( C_7[n] \).

**Table 1. The values of ABC index for some \( C_5[n] \)**

<table>
<thead>
<tr>
<th>The types of nanocones</th>
<th>The number of edges of type ( d(u)=3 ), ( d(v)=3 )</th>
<th>The number of edges of type ( d(u)=2 ), ( d(v)=2 )</th>
<th>The number of edges of type ( d(u)=3 ), ( d(v)=2 )</th>
<th>ABC index values</th>
</tr>
</thead>
<tbody>
<tr>
<td>( C_5[1] )</td>
<td>10</td>
<td>5</td>
<td>10</td>
<td>17.27</td>
</tr>
<tr>
<td>( C_5[2] )</td>
<td>35</td>
<td>5</td>
<td>20</td>
<td>41.01</td>
</tr>
<tr>
<td>( C_5[3] )</td>
<td>75</td>
<td>5</td>
<td>30</td>
<td>74.75</td>
</tr>
<tr>
<td>( C_5[4] )</td>
<td>130</td>
<td>5</td>
<td>40</td>
<td>118.5</td>
</tr>
<tr>
<td>( C_5[5] )</td>
<td>200</td>
<td>5</td>
<td>50</td>
<td>172.2</td>
</tr>
<tr>
<td>( C_5[10] )</td>
<td>775</td>
<td>5</td>
<td>100</td>
<td>590.9</td>
</tr>
<tr>
<td>( C_5[12] )</td>
<td>1110</td>
<td>5</td>
<td>120</td>
<td>828.4</td>
</tr>
<tr>
<td>( C_5[20] )</td>
<td>3050</td>
<td>5</td>
<td>200</td>
<td>2178.3</td>
</tr>
</tbody>
</table>

**Table 2. The values of ABC index for some \( C_7[n] \)**

<table>
<thead>
<tr>
<th>The types of nanocones</th>
<th>The number of edges of type ( d(u)=3 ), ( d(v)=3 )</th>
<th>The number of edges of type ( d(u)=2 ), ( d(v)=2 )</th>
<th>The number of edges of type ( d(u)=3 ), ( d(v)=2 )</th>
<th>ABC index values</th>
</tr>
</thead>
<tbody>
<tr>
<td>( C_7[1] )</td>
<td>14</td>
<td>7</td>
<td>14</td>
<td>24.18</td>
</tr>
<tr>
<td>( C_7[2] )</td>
<td>49</td>
<td>7</td>
<td>28</td>
<td>57.42</td>
</tr>
<tr>
<td>( C_7[3] )</td>
<td>105</td>
<td>7</td>
<td>42</td>
<td>104.7</td>
</tr>
<tr>
<td>( C_7[4] )</td>
<td>182</td>
<td>7</td>
<td>56</td>
<td>165.9</td>
</tr>
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<td>( C_7[5] )</td>
<td>280</td>
<td>7</td>
<td>70</td>
<td>241.1</td>
</tr>
<tr>
<td>( C_7[10] )</td>
<td>1085</td>
<td>7</td>
<td>140</td>
<td>827.3</td>
</tr>
<tr>
<td>( C_7[12] )</td>
<td>1554</td>
<td>7</td>
<td>168</td>
<td>1159.5</td>
</tr>
<tr>
<td>( C_7[20] )</td>
<td>4270</td>
<td>7</td>
<td>280</td>
<td>3049.6</td>
</tr>
</tbody>
</table>

3. An Algorithm for ABC Index

In this section, an algorithm (pseudocode) is proposed for the evaluation of the atom bond connectivity index. In algorithm, we use some variables which we defined below:
\( m \) is the number of edges of the chemical graph,
\( e_1, e_2, \ldots, e_m \) (\( e=uv \)) are the edges of the chemical graph,
\( Sum \) is the sum of ABC index for each edge.

**Step 0.** Start.
**Step 1.** Take \( Sum=0 \), \( i=0 \).
Step 2. \(i = i + 1\).
Step 3. Determine the degrees of \(d(u)\) and \(d(v)\) for \(e_i\).
Step 4. \(\text{Sum} = \text{Sum} + \sqrt{(d(u) + d(v) - 2)/(d(u)d(v))}.\)
Step 5. If \(i < m\) then, return to Step 2.
Step 6. Else, write the Sum.
Step 7. Stop.

4. Conclusion

In this paper, atom bond connectivity index of pentagonal and heptagonal carbon nanocones has been calculated and also, the theorem has been given for the first time. It is possible to apply any families of carbon nanocones. Furthermore, the algorithm can be used other vertex based topological indices. Atom bond connectivity index is convenient for measuring (connected) nanostructures which is based on degrees of their vertices.

References