The edge version of MEC index of one-pentagonal carbon nanocones

A. Nejati, M. Alaeiyan*

Department of Mathematics, College of Basic Sciences, Karaj Branch, Islamic Azad University, Alborz, Iran

Received June 27, 2013; Revised January 8, 2014

Let \( G \) be a molecular graph, the edge modified eccentric connectivity index of \( G \) is defined as

\[
\Lambda_e(G) = \sum_{f \in E(G)} S_f \cdot \text{ecc}(f),
\]

where \( S_f \) is the sum of the degrees of neighborhoods of an edge \( f \) and \( \text{ecc}(f) \) is its eccentricity. In this paper an exact formula for the edge modified eccentric connectivity index of one-pentagonal carbon nanocones was computed.

**Keywords:** edge modified eccentric connectivity index, carbon nanocones, eccentricity

**INTRODUCTION**

Molecular descriptors are playing significant role in chemistry, pharmacology, etc. Among them, topological indices have a prominent place [15]. There are numerous topological descriptors that have found some applications in theoretical chemistry, especially in QSAR/QSPR research.

More recently, a new topological index, eccentric connectivity index, has been investigated. This topological model has been shown to give a high degree of predictability of pharmaceutical properties, and may provide leads for the development of safe and potent anti-HIV compounds. We encourage the reader to consult papers [1–9] for some applications and papers [10–14] for the mathematical properties of this topological index.

One-pentagonal carbon nanocones, Fig. 1, were originally discovered by Ge and Sattler in 1994 [17]. These are constructed from a graphene sheet by removing a 60° wedge and joining the edges thus producing a cone with a single pentagonal defect at the apex. One-pentagonal carbon nanocones consist of one pentagon, its core surrounded by layers of hexagons. If there are \( n \) layers, then the graph of this molecule is denoted by \( G = \text{CNC}_5[n] \).

Now, we introduce some notation and terminology. Let \( G \) be a graph with vertex set \( V(G) \) and edge set \( E(G) \). Let \( \text{deg}(v) \) denote the degree of the vertex \( v \) in \( G \). If \( \text{deg}(v) = 1 \), then \( v \) is said to be a pendant vertex. An edge incident to a pendant vertex is said to be a pendant edge. For two vertices \( u \) and \( v \) in \( V(G) \), we denote by \( d(u,v) \) the distance between \( u \) and \( v \), i.e., the length of the shortest path connecting \( u \) and \( v \). The eccentricity of a vertex \( v \) in \( V(G) \), denoted by \( \text{ecc}(v) \), is defined as

\[
\text{ecc}(v) = \max \{d(u,v) | u \in V(G)\}
\]

The diameter of a graph \( G \) is then defined to be \( \max \{\text{ecc}(v) | v \in V(G)\} \). The eccentric connectivity index, \( \xi^c(G) \), of a graph \( G \) is defined as

\[
\xi^c(G) = \sum_{v \in V(G)} \text{deg}(v) \cdot \text{ecc}(v)
\]

The modified eccentric connectivity index of \( G \) is defined as \( \Lambda(G) = \sum_{v \in V(G)} S_v \cdot \text{ecc}(v) \), where \( S_v \) is the sum of the degrees of neighborhoods of an edge \( f \) and \( \text{ecc}(f) \) is its eccentricity.

Let \( f = uv \) be an edge in \( E(G) \). Then the degree of the edge \( f \) is defined as \( \text{deg}(u) + \text{deg}(v) - 2 \). For two edges \( f_1 = u_1v_1, f_2 = u_2v_2 \) in \( E(G) \), the distance between \( f_1 \) and \( f_2 \), denoted by \( d(f_1,f_2) \), is defined to be

\[
d(f_1,f_2) = \min \{d(u_1,u_2),d(u_1,v_2),d(v_1,u_2),d(v_1,v_2)\}
\]

The eccentricity of an edge \( f \), denoted by \( \text{ecc}(f) \), is defined as

\[
\text{ecc}(f) = \max \{d(f,e) | e \in E(G)\}
\]

The edge eccentric connectivity index of \( G \) [16], denoted by \( \xi^c_e(G) \), is defined as

\[
\xi^c_e(G) = \sum_{f \in E(G)} \text{deg}(f) \cdot \text{ecc}(f)
\]

Also the edge modified eccentric connectivity index of \( G \) is defined as \( \Lambda_f(G) = \sum_{f \in E(G)} S_f \cdot \text{ecc}(f) \), where \( S_f \) is the sum of the degrees of neighborhoods of an edge \( f \) and
In this paper an exact formula for the edge modified eccentric connectivity index of one-pentagonal carbon nanocones was computed.

RESULTS AND DISCUSSION

Let \( C[n] = \text{CNC}_5[n] \). In the following lemma, the maximum and minimum edge eccentric connectivity of \( C[n] \) is computed.

\[ \text{Max}(ecc(f)) = 4n + 1, \]
\[ \text{Min}(ecc(f)) = 2n + 1. \]

**Lemma 1.** For any edge \( f \) in \( E(C[n]) \), we have

**Proof.** Suppose \( f \) is an edge of the central pentagon of \( C[n] \). Then from Fig. 1, one can see that there exists an edge \( g \) of degree 2 such that \( d(f, g) = 2n \) and there exists another edge \( h \) of degree 2 such that \( d(f, h) = 2n + 1 \). Therefore, the shortest path with maximum length is connecting two edges of degree 2 in \( C[n] \) and thus the proof is completed.

In the following theorem we compute the edge eccentric connectivity index of \( C[n] \).

**Theorem 1.** The edge modified eccentric connectivity index of \( C[n] \) is computed as

\[ \Lambda_e(C[n]) = 400n^3 + 520n^2 + 180n + 20. \]

**Proof.** Considering Figs. 1 and 2, it can be seen that we have 10\( n+5 \) numbers of edges with maximum eccentric connectivity, such as 5 numbers of edges type 1, 10 numbers of edges type 2 and 10\( n-10 \) numbers of edges type 3. Also 5\( n \) numbers of edges type 4 with eccentric connectivity of 4, 10\( n-5 \) numbers of edges type 5 with eccentric connectivity of 4\( n-1 \), and so it continues until we have five edges of type 2\( n+2 \) with eccentric connectivity of 2\( n+2 \) and five edges of type 2\( n+3 \) with minimum eccentric connectivity of 2\( n+1 \). It is easy to check that the sum of the degrees of neighborhoods of five edges of maximum eccentric connectivity is 6. The sum of the degrees of neighborhoods of 10 edges of maximum eccentric connectivity is 9 and the sum of the degrees of neighborhoods of 10\( n-10 \) edges of maximum eccentric connectivity is 10. Also the sum of the degrees of neighborhoods of 5\( n \) edges of type 4 is 14. On the other hand, the sum of the degrees of neighborhoods of other types of edges is 16. (See Table 1).

**Table 1.** Types of edges for \( C[n] \)

<table>
<thead>
<tr>
<th>Types of edges</th>
<th>Num</th>
<th>Ecc</th>
<th>( S_f )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>5</td>
<td>4n+1</td>
<td>6</td>
</tr>
<tr>
<td>2</td>
<td>10</td>
<td>4n+1</td>
<td>9</td>
</tr>
<tr>
<td>3</td>
<td>10( n-10 )</td>
<td>4n+1</td>
<td>10</td>
</tr>
<tr>
<td>4</td>
<td>5( n )</td>
<td>4n</td>
<td>14</td>
</tr>
<tr>
<td>5</td>
<td>10( n-5 )</td>
<td>4n-1</td>
<td>16</td>
</tr>
<tr>
<td>6</td>
<td>5( n-5 )</td>
<td>4n-2</td>
<td>16</td>
</tr>
<tr>
<td>7</td>
<td>10( n-15 )</td>
<td>4n-3</td>
<td>16</td>
</tr>
<tr>
<td>8</td>
<td>5( n-10 )</td>
<td>4n-4</td>
<td>16</td>
</tr>
<tr>
<td>9</td>
<td>10( n-25 )</td>
<td>4n-5</td>
<td>16</td>
</tr>
<tr>
<td>...</td>
<td>...</td>
<td>...</td>
<td>...</td>
</tr>
<tr>
<td>2n</td>
<td>10</td>
<td>2n+4</td>
<td>16</td>
</tr>
<tr>
<td>2n+1</td>
<td>15</td>
<td>2n+3</td>
<td>16</td>
</tr>
<tr>
<td>2n+2</td>
<td>5</td>
<td>2n+2</td>
<td>16</td>
</tr>
<tr>
<td>2n+3</td>
<td>5</td>
<td>2n+1</td>
<td>16</td>
</tr>
</tbody>
</table>

This implies that

\[ \Lambda_e(C[n]) = \sum_{f \in E(C[n])} S_f \cdot ecc(f) \]
A. Nejati and M. Alaeiyan: The Edge Version of MEC Index of One-Pentagonal Carbon Nanocones

\[ n = 5 \times 6 \times (4n + 1) + 10 \times 9 \times (4n + 1) + \left( 10n - 10 \right) \times 10 \times (4n + 1) + 5n \times 14 \times 4n + 16 \sum_{k=1}^{n} \left( 10n - 10k + 5 \right) (4n - 2k + 1) + 16 \sum_{k=1}^{n-1} (5n - 5k) (4n - 2k) \]

Therefore,
\[ \Lambda_e(C(n)) = 400n^3 + 520n^2 + 180n + 20 \]

Thus, this proof is completed.

REFERENCES
12. X. Xu, The eccentric connectivity index of trees of given order and matching number (Submitted for publication).