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A Numerical Method for MEC Polynomial and MEC Index of One-Pentagonal Carbon Nanocones

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A Numerical Method for MEC Polynomial and MEC Index of One-Pentagonal Carbon Nanocones

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The modified eccentric connectivity (MEC) polynomial of a molecular graph, G, is defined as $\Lambda(G,x) = \sum_{u \in V(G)} n_G(u) x^{ecc(u)}$, where $ecc(u)$ is defined as the length of a maximal path connecting $u$ to another vertex of molecular graph $G$ and $n_G(u)$ is the sum of the degrees of its neighborhoods. The MEC index is the first derivative of this polynomial for $x = 1$. The pentagonal carbon nanocones are constructed from a graphene sheet by removing a $60^\circ$ wedge and joining the edges produces a cone with a single pentagonal defect at the apex. In this paper, we determine a numerical method for computing MEC polynomial and MEC index of one-pentagonal carbon nanocones.

Keywords MEC index, MEC polynomial, one-pentagonal carbon nanocone, Matlab program

1. Introduction

In recent years, nanostructures involving carbon have been the focus of an intense research activity, which has been driven to a large extent by the quest for new materials with specific applications. One pentagonal carbon nanocone originally discovered by Ge and Sattler in 1994 (6). These are constructed from a graphene sheet by removing a $60^\circ$ wedge and joining the edges, producing a cone with a single pentagonal defect at the apex. If a $120^\circ$ wedge is considered, then a cone with a single square defect at the apex is obtained. The case of $240^\circ$ wedge yields a single triangle defect at the apex (9,13,14,17,18,19,20). In Figure 1, one can see two types of one-pentagonal carbon nanocones (top and side view, respectively).

Topological indices are graph invariants and are used for quantitative structure-activity relationship (QSAR) and quantitative structure-property relationship (QSPR) (see ref. 4,10). Many topological indices have been defined and several applications of them have been found in physical, chemical and pharmaceutical models and other properties of molecules. A topological index of a molecular graph $G$ is a numeric quantity related to $G$. The oldest nontrivial topological index is the Wiener index which was introduced by Harold Wiener (5,11). John Platt was the only person who immediately realized the importance of the Wiener’s pioneering work and wrote papers analyzing and interpreting...
the physical meaning of the Wiener index. The name of topological index was introduced by Hosoya (1,2,3,7,8). Now some algebraic definitions are recalled that will be used in the paper. Let $G$ be a simple molecular graph without directed and multiple edges and without loops, the vertex and edge-sets of which are represented by $V(G)$ and $E(G)$, respectively. The vertices in $G$ are connected by an edge if there exists an edge $uv \in E(G)$ connecting the vertices $u$ and $v$ in $G$ so that $u, v \in V(G)$. In chemical graphs, the vertices of the graph correspond to the atoms of the molecule, and the edges represent the chemical bonds. The number of vertices and edges in a graph will be defined by $|V(G)|$ and $|E(G)|$, respectively. In graph theory, a path of length $n$ in a graph is a sequence of $n+1$ vertices such that from each of its vertices there is an edge to the next vertex in the sequence. For two vertices $x$ and $y$ of $G$, $d_G(x,y)$ denotes the length of a minimal path connecting $x$ and $y$ (Figure 1).

The eccentric connectivity index of the molecular graph, $G$, $\xi^e(G)$, was proposed by Sharma, Goswami and Madan (15,16). It is defined as $\xi^e(G) = \sum_{u \in V(G)} \text{deg}_G(u) \cdot \text{ecc}(u)$ where $\text{deg}_G(u)$ denotes the degree of the vertex $u$ in $G$ and $\text{ecc}(u) = \max\{d(x,u) \mid x \in V(G)\}$. The radius and diameter of $G$ are defined as the minimum and maximum eccentricity among vertices of $G$, respectively (2–12). The modified eccentric connectivity polynomial (MEC) of graph $G$ is defined as $\Lambda(G,x) = \sum_{u \in V(G)} n_G(u)x^{\text{ecc}(u)}$, where $n_G(u)$ is the sum of the degrees of its neighborhoods (2).
As a result, MEC index is the first derivative of this polynomial for \( x = 1 \), that is \( \Lambda(G) = \sum_{u \in V(G)} n_G(u) \cdot \text{ecc}(u) \). For example, if \( C_n \) denotes the cycle graph on \( n \) vertices, then, for every \( v \in V(C_n) \), \( \deg(v) = 2 \). One can see \( \text{ecc}(v) = \frac{n}{2} \) when \( n \) is even and \( \text{ecc}(v) = \frac{n - 1}{2} \) when \( n \) is odd. Hence,

\[
\Lambda(C_n, x) = \begin{cases} 
4nx^2 & n \text{ is even} \\
4nx^{\frac{n-1}{2}} & n \text{ is odd}
\end{cases}
\]

\[
\Lambda(C_n) = \begin{cases} 
2n^2 & n \text{ is even} \\
2n(n - 1) & n \text{ is odd}
\end{cases}
\]

2. Results and Discussion

A graph \( G \) is called connected, if there is a path connecting vertices \( x \) and \( y \) of \( G \), for every \( x, y \in V(G) \). Suppose \( X \) is a set, \( X_i \), \( 1 \leq i \leq m \), are subsets of \( X \) and \( F = \{X_i\}_{1 \leq i \leq m} \) is a family of subsets of \( X \). If \( X_i \)'s are non-empty, \( X = \bigcup_{i=1}^{m} X_i \) and \( X_i \cap X_j = \emptyset \), for \( i \neq j \) then \( F \) is called a partition of \( X \). If \( G \) is not connected then \( G \) can be partitioned into some connected subgraphs, which is called components of \( G \). Here a subgraph \( H \) of a graph \( G \) is a graph such that \( V(H) \subseteq V(G) \) and \( E(H) \subseteq E(G) \). A subgraph \( H \) of \( G \) is called isometric if for every \( x, y \in V(H) \), \( d_H(x, y) = d_G(x, y) \). In this section we calculate the MEC indices and MEC polynomials of one-pentagonal carbon nanocones by an algebraic method. In continue a Matlab program is presented which is useful for computing the MEC index and MEC polynomial of a nanocone. We apply this program to compute of the molecular graph of nanocone CNC\(_5\)[n], when \( 1 \leq n \) (see Figure 1). In this way the one-pentagonal carbon nanocones are divided into several parts of the same. Calculations are done for a section and then generalized to the total carbon. Thus we determine maximum and minimum eccentric connectivity for every section of one-pentagonal carbon nanocone with respect (Figure 2). Finally, the vertices set with same eccentric are determined (see Figure 3).

**Lemma 1.** The number of vertices and edges in a molecular graph CNC\(_5\)[n] is given by:

\[
|V(\text{CNC}_5[n])| = 5(1 + 1 + 2 + 2 + 3 + 3 + \ldots + (n - 1) + (n - 1) + n) = 5n^2 \text{ and}
\]

\[
|E(\text{CNC}_5[n])| = 5(1 + 4 + 7 + 10 + \ldots + (3n - 5) + (3n - 2)) = \frac{5}{2}(3n^2 - n)
\]

**Lemma 2.** For \( u \in V(\text{CNC}_5[n]) \), we have Max ecc\((u) = 4n-2 \) and Min ecc\((u) = 2n \).

**Proof.** Suppose \( u \) is a vertex of the central pentagon of CNC\(_5\)[n]. Then from Figure 2 one can see that there exists a vertex \( v \) of degree 2 such that \( d(u, v) = 2n \), and there exists another vertex \( w \) of degree 2 such that \( d(u, w) = 2n-2 \). Therefore, the shortest path with maximum length is connecting two vertices of degree 2 in CNC\(_5\)[n]. Then this proof is complete.

**Theorem 1.** The MEC polynomial of one-pentagonal carbon nanocone is computed as follows:

\[
\Lambda(\text{CNC}_5[n], x) = 5n(6x^2 + 7x + 9)x^{4(n-1)} - 5(2x^2 + 7x + 9)x^{4(n-1)}
\]

\[
+ \frac{45(1 + x)x^n}{x^2} \sum_{i=2}^{n-1} \frac{n - i}{x^{2i}}
\]
Proof. Suppose \( Q[n] = \text{CNC}_5[n] \). With respect to Figure 2, \( Q[n] = \bigcup_{i=1}^{5} T_i \), where \( \{T_i\}_{1 \leq i \leq 5} \) is a partition of the molecular graph \( Q[n] \). It can be seen that, the maximum eccentric connectivity for vertices type 1 and vertices type 2 with two numbers and \( n-2 \) numbers, respectively. With respect to Figure 3, we have maximum eccentric connectivity for two numbers of vertices type 1 and \( n-1 \) numbers of vertices type 2. Also \( n-1 \) numbers of vertices type 3 with eccentric connectivity equals to \( 4n-3 \), \( n-1 \) numbers of vertices type 4 with eccentric equals to \( 4n-4 \), and so it continues until we have one vertex of type \( 2n-1 \) with eccentric \( 2n+1 \) and one vertex of type \( 2n \) with minimum eccentric \( 2n \). It is easy to check that, \( \text{deg}(u) = 2 \) for vertices with maximum eccentric connectivity and \( \text{deg}(u) = 3 \) for other vertices of \( T_1 \). See Table 1 for vertices of \( T_1 \).

This implies that

\[
A(T_1, X) = \sum_{\mu \in V(T_1)} n_G(\mu) x^{ecc(\mu)} = (6n - 2)x^{4n-2} + 7(n-1)x^{4n-3} + 9(n-1)x^{4n-4} + 9(n-2)x^{4n-5} + 9(n-2)x^{4n-6} + \ldots + 9 \times 2x^{2n+3} + 9 \times 2x^{2n+2} + 9x^{2n+1} + 9^{2n} \\
= (6n - 2)x^{4n-2} + (n-1)(7x + 9)x^{4n-4} + 9(n-2)(1+x)x^{4n-6} + \ldots + 9 \times 2(1+x)x^{2n+2} + 9(1+x)x^{2n} \\
= (6n - 2)x^{4n-2} + (n-1)(7x + 9)x^{4n-4} + 9(1+x)x^{4n-6} \sum_{i=2}^{n-1} \frac{n-i}{\chi^{3i}}
\]
Figure 3. The vertices set with same eccentric connectivity for one section in CNC$_5$[7]: • Vertex with maximum eccentric connectivity; ■ Vertex with minimum eccentric connectivity.

Table 1
Types of $T_1$ Vertices for CNC$_5$[n]

<table>
<thead>
<tr>
<th>Vertices Type</th>
<th>No.</th>
<th>Ecc.</th>
<th>$n_G(u)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Vertices Type 1</td>
<td>2</td>
<td>$4n-2$</td>
<td>5</td>
</tr>
<tr>
<td>Vertices Type 2</td>
<td>$n-2$</td>
<td>$4n-2$</td>
<td>6</td>
</tr>
<tr>
<td>Vertices Type 3</td>
<td>$n-1$</td>
<td>$4n-3$</td>
<td>7</td>
</tr>
<tr>
<td>Vertices Type 4</td>
<td>$n-1$</td>
<td>$4n-4$</td>
<td>9</td>
</tr>
<tr>
<td>Vertices Type 5</td>
<td>$n-2$</td>
<td>$4n-5$</td>
<td>9</td>
</tr>
<tr>
<td>Vertices Type 6</td>
<td>$n-2$</td>
<td>$4n-6$</td>
<td>9</td>
</tr>
<tr>
<td>Vertices Type 7</td>
<td>$n-3$</td>
<td>$4n-7$</td>
<td>9</td>
</tr>
<tr>
<td>...</td>
<td>...</td>
<td>...</td>
<td>...</td>
</tr>
<tr>
<td>Vertices Type 2n−3</td>
<td>2</td>
<td>$2n+3$</td>
<td>9</td>
</tr>
<tr>
<td>Vertices Type 2n−2</td>
<td>2</td>
<td>$2n+2$</td>
<td>9</td>
</tr>
<tr>
<td>Vertices Type 2n−1</td>
<td>1</td>
<td>$2n+1$</td>
<td>9</td>
</tr>
<tr>
<td>Vertices Type 2n</td>
<td>1</td>
<td>$2n$</td>
<td>9</td>
</tr>
</tbody>
</table>
Therefore,

\[
\Lambda(Q[n], X) = \sum_{u \in V(Q[n])} n_G(u) x^{ecc(u)} = 5 \times \Lambda(T_1, X) = 5 \times \sum_{u \in V(T_1)} n_G(u) x^{ecc(u)}
\]

\[
= 5(6n - 2)x^{4n-2} + 5(n - 1)(7x + 9)x^{4n-4} + 45(1 + x)x^{4n-2} \sum_{i=2}^{n-1} \frac{n - i}{x^{2i}}
\]

\[
= 5\left(6x^2 + 7x + 9\right)n - 5\left(2x^2 + 7x + 9\right) \times x^{4n} + 45(1 + x)x^{4n} \times \sum_{i=2}^{n-1} \frac{n - i}{x^{2i}}
\]

Then this proof is completed.

**Theorem 2.** The MEC index of one-pentagonal carbon nanocone is computed as follows:

\[
\Lambda(CNC_5[n]) = 150n^3 - \frac{335}{2}n^2 + \frac{135}{2}n - 10
\]

**Proof.** From the definitions, we have \(\Lambda(CNC_5[n]) = \frac{\partial \left( \Lambda(CNC_5[n], x) \right)}{\partial x} \bigg|_{x=1}\). So we have

\[
\frac{\partial}{\partial x} \left( 5n \left(6x^2 + 7x + 9\right)x^{4(n-1)} - 5\left(2x^2 + 7x + 9\right)x^{4(n-1)} + \frac{45(1 + x)x^{4n}}{x^2} \sum_{i=2}^{n-1} \frac{n - i}{x^{2i}} \right)
\]

\[
= 5(6n - 2)(4n - 2) + 35(n - 1)(4n - 3) + 180(n - 1)^2
\]

\[
+ \sum_{i=2}^{n-1} 18(n - i)(4n - 2i - 2) + \sum_{i=2}^{n-1} 9(n - i)
\]

\[
= 5(88n^2 - 141n + 61) + 5 \left(30n^3 - \frac{243}{2}n^2 + \frac{309}{2}n - 63\right)
\]

\[
= 150n^3 - \frac{335}{2}n^2 + \frac{135}{2}n - 10
\]

Then this proof is completed.

Following is a Matlab program for computing the MEC polynomial and MEC index of one-pentagonal carbon nanocones:

```matlab
function [varargout] = lambdacnc5(varargin)
% cnc5(1:10,'plot',
%     'LimitN',[1 3 4 5],
%     'Axis',[x_min x_max y_min y_max],
%     'Grid')
nn = varargin{1};
syms x
if ischar(varargin{1}) == 1
    error('Error : Vector must have 1 Argument.')
else
    nn = varargin{1};
```
nn2 = nn;
end
F_P = strcmp(varargin,’Limit’); if sum(F_P) ≈ 0; nn2 = varargin{find(F_P)+1}; end
if size(nn,1) ≈ 1
    error(’Error: Vector(N) must have 1 row.’)
else (min(nn) < 1)
    error(’Error: N >= 1 ’)
elseif (min(nn2) < min(nn)) || (max(nn2) > max(nn))
    error(’Error: N2 ’)
else
    %%%% Eccentric Connectivity Polynomial
    for j = 1:length(nn)
        n = nn(j);
        Sigma = sum([0 ((n-(2:n-1))./(x.ˆ(2.∗(2:n-1))))]);
        ANS.MCPx(n-nn(1)+1) = ((5∗n)*((6∗(xˆ2))+(7∗x)+9)*(x’(4∗(n-1))))- . . .
        (5∗((2∗(xˆ2)+7∗x)+9)*(x’(4∗(n-1))))+((45∗(1+x)*(x’(4∗n)))/(x’2)))*Sigma;
        ANS.MCPi(n-nn(1)+1) = (150∗(nˆ3))-((335/2)∗(nˆ2))+((135/2)∗n)-10;
    end
if nargout <= 1
    varargout{1}.MCPx = ANS.MCPx ; ANS.MCPxNAME = ‘.MCPx’;
    varargout{1}.MCPi = ANS.MCPi ; ANS.MCPiNAME = ‘.MCPi’;
else
    varargout{1} = ANS.MCPx ; ANS.MCPxNAME = ‘ARG1’;
    varargout{2} = ANS.MCPi ; ANS.MCPiNAME = ‘ARG2’;
end
%%%% Plot
F_P = strcmp(varargin,’plot’);
if sum(F_P) ≈ 0
    clf
    subplot(1,3,1:2)
    hold on
    for i = 1:length(nn2)
        set(gca,’ColorOrder’,[rand(1) rand(1) rand(1)])
        ezplot(ANS.MCPx(nn2(i)-nn(1)+1))
    end
    F_P = strcmp(varargin,’Grid’) ; if sum(F_P) ≈ 0 ; set(gca,’YGrid’,’on’) ; end
    hold off
    F_P = strcmp(varargin,’Axis’) ; if sum(F_P) ≈ 0 ; axis(varargin{find(F_P)+1}) ; end
if length(nn2) == 1; Y_S = ’’; else Y_S = ’s’ ; end
if length(nn2) ≈ length(nn) || length(nn) == 1
    if size(nn2,2) <= 5 ; T_mat1 = nn2 ; T_S = ’ ’ ; T_mat2 = ’ ’ ;
    else T_S = ’ . . ’ ; T_mat1 = nn2(1:3) ; T_mat2 = nn2(length(nn2)-1:end) ; end
    title([’\lambda (CNC_{5}[n],x) n = ’ num2str(T_mat1) T_S num2str(T_mat2)]);
    ylabel([num2str(length(nn2)) ’ Function’ Y_S])
    xlabel(’Modified Eccentric Connectivity Polynomial’)
    subplot(1,3,3),bar(nn2,ANS.MCPi(nn2-nn(1)+1))
    axis([min(nn2)-1 max(nn2)+1 0 max(ANS.MCPi)+1])
In Tables 2 and 3, we calculate the MEC polynomials and MEC indices of CNC₅ₙ for 1≤n≤10, respectively. In Figures 4 and 5, the diagrams of the MEC Polynomials

<table>
<thead>
<tr>
<th>One-pentagonal carbon nanocones</th>
<th>Modified eccentric connectivity polynomials</th>
</tr>
</thead>
<tbody>
<tr>
<td>CNC₅₁</td>
<td>20x²</td>
</tr>
<tr>
<td>CNC₅₂</td>
<td>50x⁶ + 35x⁴ + 45x⁴</td>
</tr>
<tr>
<td>CNC₅₃</td>
<td>80x¹⁰ + 70x⁴ + 90x⁸ + 45x⁶ + 45x⁶</td>
</tr>
<tr>
<td>CNC₅₄</td>
<td>110x¹⁴ + 105x¹³ + 135x¹² + 90x¹¹ + 90x¹⁰ + 45x⁹ + 45x⁸</td>
</tr>
<tr>
<td>CNC₅₅</td>
<td>140x¹⁸ + 140x¹⁷ + 180x¹⁶ + 135x¹⁵ + 135x¹⁴ + 90x¹³ + 90x¹² + 45x¹¹ + 45x¹⁰</td>
</tr>
<tr>
<td>CNC₅₆</td>
<td>170x²² + 175x²¹ + 225x²⁰ + 180x¹⁹ + 180x¹⁸ + 135x¹⁷ + 135x¹⁶ + 90x¹⁵ + 90x¹⁴ + 45x¹³ + 45x¹²</td>
</tr>
<tr>
<td>CNC₅₇</td>
<td>200x²⁶ + 210x²⁵ + 270x²⁴ + 225x²³ + 225x²² + 180x²¹ + 180x²⁰ + 135x¹⁹ + 135x¹⁸ + 90x¹⁷ + 90x¹⁶ + 45x¹⁵ + 45x¹⁴</td>
</tr>
<tr>
<td>CNC₅₈</td>
<td>230x³⁰ + 245x²⁹ + 315x²⁸ + 270x²⁷ + 270x²⁶ + 225x²⁵ + 225x²⁴ + 180x²³ + 180x²² + 135x²¹ + 135x²⁰ + 90x¹⁹ + 90x¹⁸ + 45x¹⁷ + 45x¹⁶</td>
</tr>
<tr>
<td>CNC₅₉</td>
<td>270x³⁴ + 280x³³ + 360x³² + 315x³¹ + 315x³⁰ + 270x²⁹ + 270x²⁸ + 225x²⁷ + 225x²⁶ + 180x²⁵ + 180x²⁴ + 135x²³ + 135x²² + 90x²¹ + 90x²⁰ + 45x²⁹ + 45x¹⁸</td>
</tr>
<tr>
<td>CNC₅₁₀</td>
<td>290x³⁸ + 315x³⁷ + 405x³⁶ + 360x³⁵ + 360x³⁴ + 315x³³ + 315x³² + 270x³¹ + 270x³⁰ + 225x²⁹ + 225x²⁸ + 180x²⁷ + 180x²⁶ + 135x²⁵ + 135x²⁴ + 90x²³ + 90x²² + 45x²¹ + 45x²⁰</td>
</tr>
</tbody>
</table>

Table 2

Some special types of MEC polynomials for CNC₅ₙ
Table 3

Some exceptional cases of MEC index for CNC₅[n]

<table>
<thead>
<tr>
<th>n</th>
<th>(\Lambda(\text{CNC}_5[n]))</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>40</td>
</tr>
<tr>
<td>2</td>
<td>655</td>
</tr>
<tr>
<td>3</td>
<td>2735</td>
</tr>
<tr>
<td>4</td>
<td>7180</td>
</tr>
<tr>
<td>5</td>
<td>14890</td>
</tr>
<tr>
<td>6</td>
<td>26765</td>
</tr>
<tr>
<td>7</td>
<td>43705</td>
</tr>
<tr>
<td>8</td>
<td>66610</td>
</tr>
<tr>
<td>9</td>
<td>96380</td>
</tr>
<tr>
<td>10</td>
<td>133915</td>
</tr>
</tbody>
</table>

Figure 4. The diagram of the MEC polynomials of CNC₅[n] (color figure available online).
and MEC indices of CNC₅[n] are depicted. The diagram of MEC polynomial is ascending and MEC index (the first derivative of MEC polynomial for at x = 1) is strictly ascending.

3. Conclusions
In this paper, we determine a numerical method for computing MEC polynomials and MEC index of one-pentagonal carbon nanocones. Our numerical method is general and also can be extended to other nanomaterials. On the other hand, by using this Matlab program modified eccentric connectivity index and polynomial for carbon nanocones of any arbitrary capacities can be calculated.

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Numerical Method for MEC Polynomial and Index

References