ON TOPOLOGICAL INDICES OF CYCLE RELATED GRAPHS

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ABSTRACT. A topological index of a graph is a numerical invariant of a chemical (molecular) graph. A molecular graph is a collection of points representing the atoms in the molecules and set of lines representing the covalent bonds. The total eccentricity polynomial of a connected graph $G$ is defined as $\text{TEP}(G, x) = \sum_{u \in V(G)} x^{\varepsilon(u)}$ where $\varepsilon(u)$ denotes the eccentricity of the vertex $u$ in $G$. In this paper total eccentricity polynomial, total eccentricity indices, eccentric connectivity indices and multiplicative Zagreb eccentricity indices are computed for some families of cycle graphs (cycloalkanes in chemical graph).

1. INTRODUCTION

Chemical graph theory is an area of mathematical chemistry which put in graph theory to mathematical modeling of the chemical phenomena [2, 11, 12]. A graph invariant is a property of graphs that depends only on the abstract structure specifically, it does not depend on the labeling or the pictorial illustration of a graph. These graph invariants are referred to as topological indices in chemical graph theory. One of the most broadly recognized topological descriptor is the Wiener index [7] specified after chemist Harold Wiener. There are some significant classes of topological indices such as distance based, eccentricity based, degree based and counting related. Let $G$ be a connected graph by means of vertex and edge sets $V(G)$ and $E(G)$ respectively. For every vertex $u \in V(G)$,
the edge connecting \( u \) and \( v \) is indicated by \( uv \) and the degree of any vertex is stands for \( d_G(u) \) (or \( d_u \)). Let the maximum and minimum degree of all the vertices of \( G \) are correspondingly denoted by \( \Delta \) and \( \delta \). The distance \( d(u, v) \) of any two vertices \( u \) and \( v \) of \( G \) is the number of edges in a shortest path connecting them. The eccentricity of a vertex is the distance of vertex \( u \) from the farthest vertex in \( G \). In other terms, \( \varepsilon(v) = \max\{d(u, v) | u \in V(G)\} \). The total eccentricity polynomial is the polynomial description of the total-eccentricity index.

**Definition 1.1.** The total eccentricity polynomial (TEP) of a graph \( G \) [8], is defined as \( \text{TEP}(G, x) = \sum_{u \in V(G)} x^{\varepsilon(u)} \) where \( \varepsilon(u) \) indicates the eccentricity of the vertex \( u \).

**Definition 1.2.** The total-eccentricity index of the graph \( G \) is defined by

\[
\zeta(G) = \sum_{u \in V(G)} \varepsilon(u).
\]

It is simple the total-eccentricity index (TEI) can be attained from the respective polynomial by assessing its first derivative at \( x = 1 \), see [1]. In recent times 2012, Nilanjan De presented a new edition of First Zagreb index [3] as the Multiplicative Zagreb Eccentricity index.

**Definition 1.3.** The multiplicative Zagreb eccentricity index is defined as

\[
\prod E_1(G) = \prod_{v \in V(G)} \varepsilon(v)^2.
\]

**Definition 1.4.** The eccentric connectivity index \( \xi(G) \) of a graph \( G \) is defined as

\[
\xi(G) = \sum_{u \in V(G)} d_u \times \varepsilon(v).
\]

This index was established by Sharma et al. in 1997 [4–6,9,10]. The intend of this paper is to examine the total eccentricity polynomial and topological indices of cycloalkanes families(cycle graphs).

2. **Results and Discussions**

2.1. **TEP and topological indices of hydrogen depleted cycloalkanes.** Hydrogen depleted cycloalkanes is cycle \( C_n \) in graph theory language. Let \( G = C_n \) be the cycle graph. Let the vertices (atoms) and edges (bonds) of \( C_n \)
Table 1. Eccentricity based indices of Cycle graphs

<table>
<thead>
<tr>
<th>G</th>
<th>Vertices</th>
<th>Eccentricity</th>
</tr>
</thead>
<tbody>
<tr>
<td>$C_3$</td>
<td>$v_1, v_2, v_3$</td>
<td>1</td>
</tr>
<tr>
<td>$C_4$</td>
<td>$v_1, v_2, v_3, v_4$</td>
<td>2</td>
</tr>
<tr>
<td>$C_5$</td>
<td>$v_1, v_2, v_3, v_4, v_5$</td>
<td>2</td>
</tr>
<tr>
<td>$C_6$</td>
<td>$v_1, v_2, v_3, v_4, v_5, v_6$</td>
<td>3</td>
</tr>
<tr>
<td>$C_7$</td>
<td>$v_1, v_2, v_3, v_4, v_5, v_6, v_7$</td>
<td>3</td>
</tr>
</tbody>
</table>

be $v_1, v_2, ..., v_n; e_1, e_2, ..., e_n$ respectively. The eccentricity of a vertex is defined as $\varepsilon(v) = \max\{d(u, v) | u \in V(G)\}$.

Total eccentricity polynomial is $\text{TEP}(G, x) = \sum_{u \in V(G)} x^{\varepsilon(u)}$.

From table 1, $\text{TEP}(C_3, x) = 3x$, $\text{TEP}(C_4, x) = 4x^2$, $\text{TEP}(C_5, x) = 5x^2$, $\text{TEP}(C_6, x) = 6x^3$ and in general $\text{TEP}(C_n, x) = n x^{\lfloor n/2 \rfloor}$. The total-eccentricity index of $G$ is $\zeta(G) = \sum_{u \in V(G)} \varepsilon(u)$. By evaluating the first derivative of its respective polynomial at $x = 1$, see [1], we can acquired it easily. From table 1, $\zeta(C_3) = 3$, $\zeta(C_4) = 8$, $\zeta(C_5) = 10$, $\zeta(C_6) = 18$ and in general, total-eccentricity index $\zeta(G) = n \lfloor n/2 \rfloor$.

The multiplicative Zagreb eccentricity index is $\prod_{v \in V(G)} E_1(v) = \prod_{v \in V(G)} \varepsilon(v)^2$. From Table 1, $\prod_{v \in V(C_3)} E_1(v) = (1^2)^3$, $\prod_{v \in V(C_4)} E_1(v) = (2^2)^4$, $\prod_{v \in V(C_5)} E_1(v) = (2^2)^5$, $\prod_{v \in V(C_6)} E_1(v) = (3^2)^6$ and hence, $\prod_{v \in V(G)} E_1(v) = \lfloor ([n/2])^2 \rfloor^n$. The eccentricity connectivity index is $\xi(G) = \sum_{v \in V(G)} d_v \times \varepsilon(v)$. From Figure 1, $\xi(C_3) = 6$, $\xi(C_4) = 16$, $\xi(C_5) = 20$ and hence $\xi(C_n) = n \left[ \frac{2}{n/2} \right]$.

2.2. TEP and topological indices of cycloalkanes (molecular structure). Figure 2. illustrates the molecular structure of cycloalkanes. $C_n \odot K_2$ in graph theory language. Let $G = C_n \odot K_2$ be a graph. Let the vertices (atoms) of $C_n \odot K_2$ be $v_1, v_2, ..., v_n; u_1, u_2, ..., u_{2n}$. In this graph $G$, $n$ vertices have eccentricity $(n-2)$ and $2n$ vertices have eccentricity $(n-1)$ and hence $\text{TEP}(C_n \odot K_2, x) = nx^{n-2} + 2nx^{n-1}$. 
From Table 2, $\text{TEP}(C_3 \odot K_2, x) = 3x + 6x^2$, $\text{TEP}(C_4 \odot K_2, x) = 4x^2 + 8x^3$, $\text{TEP}(C_5 \odot K_2, x) = 5x^3 + 10x^4$ and in general $\text{TEP}(C_n \odot K_2, x) = nx^{n−2} + 2nx^{n−1}$. Here the total-eccentricity indices are $\zeta(C_3 \odot K_2) = 15$, $\zeta(C_4 \odot K_2) = 32$, $\zeta(C_5 \odot K_2) = 10$, $\zeta(C_6 \odot K_2) = 55$ and hence $\zeta(G) = 3n^2 − 4n$. The multiplicative Zagreb eccentricity index of $C_n \odot K_2$ is $\prod E_1(C_n \odot K_2) = [(n−2)^2]^n [(n−2)^2]^{2n}$. From
Figure 2, eccentricity connectivity index \( \xi(C_3 \odot K_2) = 24 \), \( \xi(C_4 \odot K_2) = 56 \), \( \xi(C_5 \odot K_2) = 100 \) and in general \( \xi(C_n \odot K_2) = 6n^2 - 10n \).

From Table 3, TEP\((C_3 \times K_2, x) = 6x^2\), TEP\((C_4 \times K_2, x) = 8x^3\), TEP\((C_5 \times K_2, x) = 10x^3\), TEP\((C_6 \times K_2, x) = 12x^4\) and so on.

In general, TEP\((C_n \times K_2, x) = 2nx^{\lfloor n/2 \rfloor + 1}, n \geq 3\). The total-eccentricity index, \( \zeta(C_3 \times K_2) = 12 \), \( \zeta(C_4 \times K_2) = 24 \), \( \zeta(C_5 \times K_2) = 30 \), \( \zeta(C_6 \times K_2) = 48 \) and hence \( \zeta(C_n \times K_2) = 2n\left(\lfloor n/2 \rfloor + 1\right) \) for \( n \geq 3 \), the multiplicative Zagreb eccentricity
The eccentric connectivity index is
\[ \zeta(C_n \times K_2) = 6n \left( \left\lfloor \frac{n}{2} \right\rfloor + 1 \right). \]

2.4. TEP and topological indices of polycyclic aromatic hydrocarbons. Figure 4 represents polycyclic aromatic hydrocarbons (PAHs) are organic compounds that are composed of multiple aromatic rings. Let \( G = C_{4n+2}, n \geq 5 \) be a PAHs graph with vertex set \( V(G) = \{v_i, v'_i, w_i, w'_i/1 \leq i \leq n+1\} \cup \{a, b, a', b'\} \) and edge set \( E(G) = \{u_i v_i, u_i v'_i, w_i v_i, w_i v'_i, v_i u_{i+1}, u_{i+1} v'_i/1 \leq i \leq n\} \cup \{u_i u'_i/1 \leq i \leq n+1\} \cup \{a u_{n+1}, b u'_{n+1}\} \cup \{a' u'_1, b' u'_1\} \). The consequent graph thus obtained is denoted as \( C_{4n+2} \) (in molecular chemistry, number of carbon atoms present in polycyclic aromatic hydrocarbons is \( 4n+2 \)) is shown in figure 4. Here \( |V(G)| = 6n + 6 \) and \( |E(G)| = 7n + 5 \). In \( G \), for odd \( n \geq 5 \), 2 vertices have eccentricity \( n + 2 \), 6 vertices have eccentricity \( n + 3 \), 4 vertices have eccentricity \( (2k - 1) \), \( k = \left( \left\lfloor \frac{n}{2} \right\rfloor + 3 \right) \) to \( n + 2 \), vertices have eccentricity \( 2k, k = \left( \left\lfloor \frac{n}{2} \right\rfloor + 3 \right) \) to \( n + 1 \) and for even \( n \geq 6 \), 2 vertices have eccentricity \( n + 2 \), 4 vertices have eccentricity \( 2k - 1 \), \( k = (n/2 + 2) \) to \( n + 2 \), 8 vertices have eccentricity \( 2k, k = (n/2 + 2) \) to \( n + 1 \). The first few total eccentricity polynomial in the first few are as follows:
\[\text{TEP}(C_{4 \times 5+2}, x) = 2x^7 + 6x^8 + 4x^9 + 8x^{10} + 4x^{11} + 8x^{12} + 4x^{13}\]
\[\text{TEP}(C_{4 \times 6+2}, x) = 2x^8 + 4x^9 + 8x^{10} + 4x^{11} + 8x^{12} + 4x^{13} + 8x^{14} + 4x^{15}\]
\[\text{TEP}(C_{4 \times 7+2}, x) = 2x^9 + 6x^{10} + 4x^{11} + 8x^{12} + 4x^{13} + 8x^{14} + 4x^{15} + 8x^{16} + 4x^{17}\]

and therefore,

\[
\text{TEP}(C_{4n+2}, x) = \begin{cases} 
2x^{n+2} + 6x^{n+3} + \sum_{k=\lceil n/2 \rceil + 1}^{n+2} 4x^{2k-1} + \sum_{k=\lceil n/2 \rceil + 1}^{n+2} 8x^{2k}, & n \geq 5 \text{ odd}, \\
2x^{n+2} + \sum_{k=n/2+2}^{n+2} 4x^{2k-1} + \sum_{k=n/2+2}^{n+1} 8x^{2k}, & n \geq 6 \text{ even}.
\end{cases}
\]

The total-eccentricity index \(\zeta(C_{4 \times 5+2}) = 382\), \(\zeta(C_{4 \times 6+2}) = 496\) and hence,

\[
\zeta(G) = \begin{cases} 
2(n + 2) + 6(n + 3) + \sum_{k=\lceil n/2 \rceil + 1}^{n+2} 4(2k - 1) + \sum_{k=\lceil n/2 \rceil + 1}^{n+2} 8(2k), & n \geq 5 \text{ odd}, \\
2(n + 2) + \sum_{k=n/2+2}^{n+2} 4(2k - 1) + \sum_{k=n/2+2}^{n+1} 8(2k), & n \geq 6 \text{ even}.
\end{cases}
\]

The multiplicative Zagreb eccentricity index of \(C_{4n+2}\) is,

\[
\Pi E_1(C_{4n+2}) = \begin{cases} 
[(n + 2)^2]^2 + [(n + 3)^2]^2 \left[ \sum_{k=\lceil n/2 \rceil + 1}^{n+2} [(2k - 1)^2]^4 \right] \sum_{k=\lceil n/2 \rceil + 1}^{n+2} [(2k)^2]^8 , & \text{for odd } n, \\
(n + 2)^2 \left[ \sum_{k=n/2+2}^{n+2} [(2k - 1)^2]^4 \right] \sum_{k=n/2+2}^{n+1} [(2k)^2]^8 , & \text{for even } n.
\end{cases}
\]
The eccentricity connectivity index is

$$\xi(C_{4n+2}) = \begin{cases} 3\left[2(n+2) + 4(n+3) + \sum_{k=\lfloor n/2 \rfloor + 3}^{n+1} 4(2k-1) + \sum_{k=\lfloor n/2 \rfloor + 3}^{n+1} 4(2k)\right] \\ +1\left[2(n+3) + \sum_{k=\lfloor n/2 \rfloor + 3}^{n+1} 4(2k) + 4(2n+3)\right] & \text{odd } n \\ 3\left[2(n+2) + \sum_{k=\lfloor n/2 \rfloor + 3}^{n+1} 4(2k-1) + \sum_{k=\lfloor n/2 \rfloor + 3}^{n+1} 4(2k)\right] \\ +1\left[\sum_{k=\lfloor n/2 \rfloor + 3}^{n+1} 4(2k) + 4(2n+3)\right] & \text{even } n \end{cases}$$

That is

$$\xi(C_{4n+2}) = \begin{cases} 3\left[(6n+16) + \sum_{k=\lfloor n/2 \rfloor + 3}^{n+1} 4(2k-1) + \sum_{k=\lfloor n/2 \rfloor + 3}^{n+1} 4(2k)\right] \\ +1\left[(10n+18) + \sum_{k=\lfloor n/2 \rfloor + 3}^{n+1} 4(2k)\right] & \text{odd } n \\ 3\left[2(n+2) + \sum_{k=\lfloor n/2 \rfloor + 3}^{n+1} 4(2k-1) + \sum_{k=\lfloor n/2 \rfloor + 3}^{n+1} 4(2k)\right] \\ +1\left[\sum_{k=\lfloor n/2 \rfloor + 3}^{n+1} 4(2k) + 4(2n+3)\right] & \text{even } n \end{cases}$$

2.5. TEP and topological indices of \([n]\) phenacene series. Figure 5. presents a \([n]\)phenacene series of hydrocarbons with \(|V(G)| = 6n+6\) and \(|E(G)| = 7n+5\). In molecular chemistry, number of carbon atoms present in \([n]\)phenacene series of hydrocarbons is \(4n+2\). Hence the graph is denoted as \(C_{4n+2}^n\). In \(G\), 4 vertices
Figure 5. \([n]\)phenacene series for \(n = 5,6\)

have eccentricity \((n + 2)\), 6 vertices have eccentricity \(k, k = (n + 3)\) to \((2n + 2)\), 2 vertices have eccentricity \((2n + 3)\).

The first few total eccentricity polynomials are as follows:

\[
\begin{align*}
\text{TEP}(C^*_4 \times 5+2, x) &= 4x^6 + 6x^7 + 6x^8 + 6x^9 + 6x^{10} + 2x^{11} \\
\text{TEP}(C^*_4 \times 6+2, x) &= 4x^7 + 6x^8 + 6x^9 + 6x^{10} + 6x^{11} + 6x^{12} + 2x^{13} \\
\text{TEP}(C^*_4 \times 7+2, x) &= 4x^8 + 6x^9 + 6x^{10} + 6x^{11} + 6x^{12} + 6x^{13} + 6x^{14} + 2x^{15}
\end{align*}
\]

and thus,

\[
\text{TEP}(C^*_4 n+2, x) = 4x^{n+2} + \sum_{k=n+3}^{2n+2} 6x^k + 2x^{2n+3}
\]

and

\[
\text{TEI} \text{ is } \zeta(G) = 4(n + 2) + \sum_{k=n+3}^{2n+2} 6k + 2(2n + 3). \text{ The multiplicative Zagreb eccentricity index of } C^*_4 n+2 \text{ is}
\]

\[
\prod E_1(C^*_4 n+2) = [(n + 2)^2]^4 \left[ \sum_{k=n+3}^{2n+2} [(k)^2]^6 \right] \left[ (2n + 3)^2 \right]^2, n \geq 4,
\]

and the eccentricity connectivity index is

\[
\xi(C^*_4 n+2).
\]

\section*{References}


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