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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 $u \in V(G)$,

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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 $\triangle$ and δ. 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 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*

$$\xi(G) = \sum_{u\in V(G)} d_v \times \varepsilon(v)\,.$$

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

G	Vertices	Eccentricity
C_3	v_1, v_2, v_3	1
C_4	v_1, v_2, v_3, v_4	2
C_5	v_1, v_2, v_3, v_4, v_5	2
C_6	$v_1, v_2, v_3, v_4, v_5, v_6$	3
C_7	$v_1, v_2, v_3, v_4, v_5, v_6, v_7$	3

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 TEP$(G,x) = \sum_{u\in V(G)} x^{\varepsilon(u)}$.

From table 1, TEP$(C_3,x) = 3x$, TEP$(C_4,x) = 4x^2$, TEP$(C_5,x) = 5x^2$, TEP$(C_6,x) = 6x^3$ and in general 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 $\prod E_1(G) = \prod_{v\in V(G)} \varepsilon(v)^2$. From Table 1, $\prod E_1(C_3) = (1^2)^3$, $\prod E_1(C_4) = (2^2)^4$, $\prod E_1(C_5) = (2^2)^5$, $\prod E_1(C_6) = (3^2)^6$ and hence, $\prod E_1(G) = [(\lfloor n/2 \rfloor)^2]^n$. 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 $\xi(C_n) = n\left[2\left\lfloor n/2 \right\rfloor\right]$.

2.2. **TEP and topological indices of cycloalkanes (molecular structure).** Figure 2. illustrates the molecular structure of cycloalkanes. $C_n \odot \overline{K_2}$ in graph theory language. Let $G = C_n \odot \overline{K_2}$ be a graph. Let the vertices (atoms) of $C_n \odot \overline{K_2}$ 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 TEP$(C_n \odot \overline{K_2}$,x$)$ = nx^{n-2} + 2nx^{n-1}.

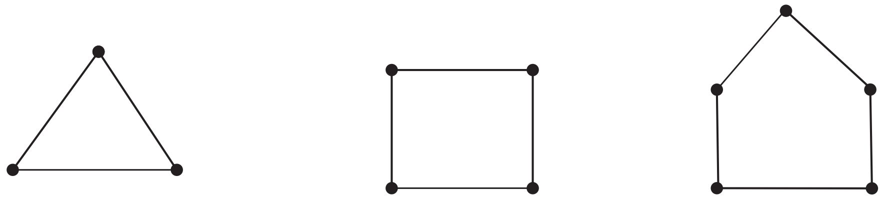


Figure1. Cycle C_n for n = 3, 4, 5, 6 (geometric structure of cycloalkanes)

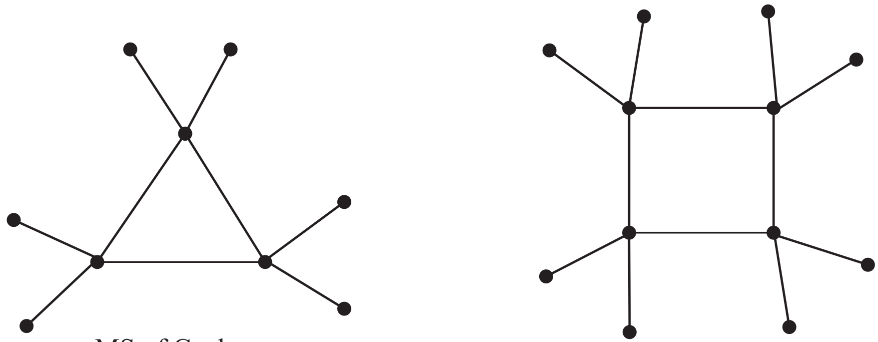


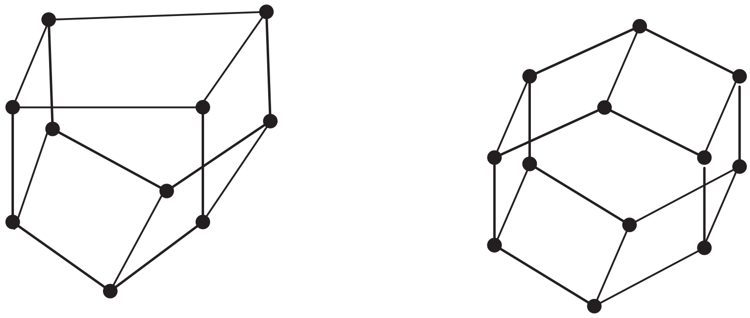
Figure 2. $C_n \odot \overline{K}_2$ for n = 3, 4, 5 (Molecular structure of cycloalkanes)

TABLE 2. Eccentricity based indices of $G = C_n \odot \overline{K_2}$

G	Vertices	Eccentricity $\varepsilon(u)$	Vertices	Eccentricity $\varepsilon(u)$
$C_3 \odot \overline{K_2}$	v_1, v_2, v_3	1	$u_1, u_2, ..., u_6$	2
$C_4 \odot \overline{K_2}$	v_1, v_2, v_3, v_4	2	$u_1, u_2, ..., u_8$	3
$C_5 \odot \overline{K_2}$	v_1, v_2, v_3, v_4, v_5	3	$u_1, u_2, ..., u_{10}$	4
$C_6 \odot \overline{K_2}$	$v_1, v_2, v_3, v_4, v_5, v_6$	4	$u_1, u_2, ..., u_{12}$	5

From Table 2, TEP($C_3 \odot \overline{K_2}, x) = 3x + 6x^2$, TEP($C_4 \odot \overline{K_2}, x) = 4x^2 + 8x^3$, TEP($C_5 \odot \overline{K_2}, x) = 5x^3 + 10x^4$ and in general TEP($C_n \odot \overline{K_2}, x) = nx^{n-2} + 2nx^{n-1}$. Here the total-eccentricity indices are $\zeta(C_3 \odot \overline{K_2}) = 15, \zeta(C_4 \odot \overline{K_2}) = 32, \zeta(C_5 \odot \overline{K_2}) = 10, \zeta(C_6 \odot \overline{K_2}) = 55$ and hence $\zeta(G) = 3n^2 - 4n$. The multiplicative Zagreb eccentricity index of $C_n \odot \overline{K_2}$ is $\prod E_1(C_n \odot \overline{K_2}) = \left[(n-2)^2\right]^n \left[(n-2)^2\right]^{2n}$. From

Figure 2, eccentricity connectivity index $\xi(C_3 \odot \overline{K_2}) = 24$, $\xi(C_4 \odot \overline{K_2}) = 56$, $\xi(C_5 \odot \overline{K_2}) = 100$ and in general $\xi(C_n \odot \overline{K_2}) = 6n^2 - 10n$.



D5R

(double 5-ring)

D6R

(double 6-ring)

Figure 3. $C_n \times K_2$ for n = 5, 6 (zeolite teritary units in molecular chemistry)

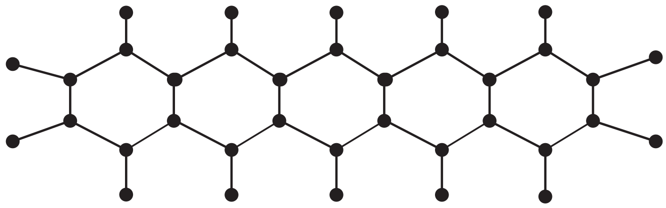
2.3. **TEP and topological indices of zeolite teritary building [n-n] units of cycloalkanes.** Figure 3. illustrates the zeolite tertiary building units of cy-coalkanes. $C_n \times K_2$ in graph theory language. Let $G = C_n \times K_2$ be a graph. Let the vertices (atoms) of $C_n \times K_2$ be $v_1, v_2, ..., v_{2n}$. In this graph G, $2n$ vertices have eccentricity $\lfloor n/2 \rfloor + 1$, for $n \geq 3$.

TABLE 3. Eccentricity based indices of $C_n \times K_2$

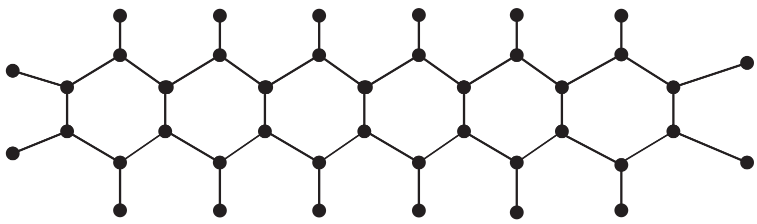
G	Vertices	Eccentricity
$C_3 \times K_2$	$v_1, v_2, ..., v_6$	2
$C_4 \times K_2$	$v_1, v_2, ..., v_8$	3
$C_5 \times K_2$	$v_1, v_2, ..., v_{10}$	3
$C_6 \times K_2$	$v_1, v_2, ..., v_{12}$	4
$C_7 \times K_2$	$v_1, v_2, ..., v_{14}$	4

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 $\zeta(C_n \times K_2) = 2n\Big(\lfloor n/2 \rfloor + 1\Big)$ for $n \geq 3$, the multiplicative Zagreb eccentricity index is $\prod E_1(C_n \times K_2) = \left[\left(\lfloor n/2 \rfloor + 1\right)^2\right]^{2n}$ for $n \geq 3$,and the eccentricity connectivity index is $\zeta(C_n \times K_2) = 6n\left[\left\lfloor n/2 \right\rfloor + 1\right]$.



pentacene: (five rings)



hexahelicene:(six rings)

Figure 4. C_{4n+2} for n = 5,6

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 $V(G) = \{v_i, v_i^{'}, w_i, w_i^{'}/1 \leq i \leq n\} \cup \{u_i, u_i^{'}/1 \leq i \leq n+1\} \cup \{a, b, a^{'}, b^{'}\}$ and edge set $E(G) = \{u_iv_i, u_iv_i^{'}, w_iv_i, w_i^{'}v_i^{'}, v_iu_{i+1}, u_{i+1}^{'}v_i^{'}/1 \leq i \leq n\} \cup \{u_iu_i^{'}/1 \leq i \leq n+1\} \cup \{au_{n+1}, bu_{n+1}^{'}\} \cup \{a^{'}u_1, b^{'}u_1^{'}\}$. 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 $\mid V(G) \mid = 6n+6$ and $\mid E(G) \mid = 7n+5$. In G, for odd $n \geq 5$, 2 vertices have eccentricity $(n+2)$, 6 vertices have eccentricity $(n+3)$, 4 vertices have eccentricity $(2k-1)$, $k = \left(\left\lfloor n/2 \right\rfloor + 3\right)$ to $(n+2)$, vertices have eccentricity $2k$, $k = \left(\left\lfloor n/2 \right\rfloor + 3\right)$ 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,

$$TEP(C_{4n+2},x)=\begin{cases} 2x^{n+2}+6x^{n+3}+\sum\limits_{k=\lfloor n/2\rfloor+3}^{n+2}4x^{2k-1}+\sum\limits_{k=\lfloor n/2\rfloor+3}^{n+2}8x^{2k}, \\ n\geq 5 \text{ odd}, \\ 2x^{n+2}+\sum\limits_{k=n/2+2}^{n+2}4x^{2k-1}+\sum\limits_{k=n/2+2}^{n+1}8x^{2k}, \\ n\geq 6 \text{ even}. \end{cases}$$

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

$$\zeta(G)=\begin{cases} 2(n+2)+6(n+3)+\sum\limits_{k=\lfloor n/2\rfloor+3}^{n+2}4(2k-1)+\sum\limits_{k=\lfloor n/2\rfloor+3}^{n+1}8(2k), \\ n\geq 5 \text{ odd}, \\ 2(n+2)+\sum\limits_{k=n/2+2}^{n+2}4(2k-1)+\sum\limits_{k=n/2+2}^{n+1}8(2k), \\ n\geq 6 \text{ even}. \end{cases}$$

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

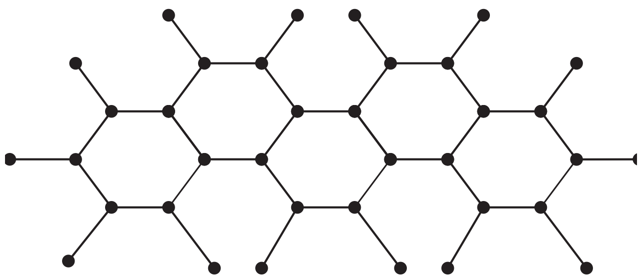
$$\prod E_1(C_{4n+2})=\begin{cases} [(n+2)^2]^2+[(n+3)^2]^6\Big[\sum\limits_{k=\lfloor n/2\rfloor+3}^{n+2}[(2k-1)^2]^4\Big]\Big[\sum\limits_{k=\lfloor n/2\rfloor+3}^{n+1}[(2k)^2]^8\Big] \\ \text{for odd } n, \\ (n+2)^2\Big[\sum\limits_{k=n/2+2}^{n+2}[(2k-1)^2]^4\Big]\Big[\sum\limits_{k=n/2+2}^{n+1}[(2k)^2]^8\Big] \\ \text{for even } n. \end{cases}$$

The eccentricity connectivity index is

$$\xi(C_{4n+2}) = \begin{cases} 3\Big[2(n+2)+4(n+3)+\sum\limits_{k=\lfloor n/2\rfloor+3}^{n+1} 4(2k-1)+\sum\limits_{k=\lfloor n/2\rfloor+3}^{n+1} 4(2k)\Big] \\ \quad +1\Big[2(n+3)+\sum\limits_{k=\lfloor n/2\rfloor+3}^{n+1} 4(2k)+4(2n+3)\Big], \text{odd} \quad n \\ 3\Big[2(n+2)+\sum\limits_{k=n/2+2}^{n+1} 4(2k-1)+\sum\limits_{k=n/2+2}^{n+1} 4(2k)\Big] \\ \quad +1\Big[\sum\limits_{k=n/2+2}^{n+1} 4(2k)+4(2n+3)\Big], \text{even} \quad n\,. \end{cases}$$

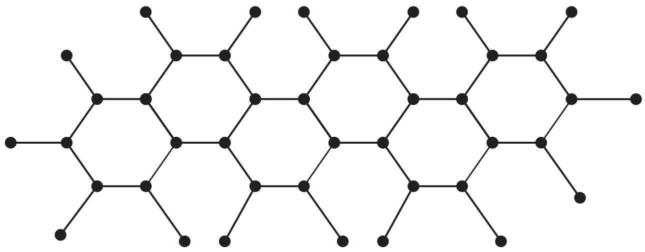
That is

$$\xi(C_{4n+2}) = \begin{cases} 3\Big[(6n+16)+\sum\limits_{k=\lfloor n/2\rfloor+3}^{n+1} 4(2k-1)+\sum\limits_{k=\lfloor n/2\rfloor+3}^{n+1} 4(2k)\Big]+ \\ 1\Big[(10n+18)+\sum\limits_{k=\lfloor n/2\rfloor+3}^{n+1} 4(2k)\Big], \text{ odd} \quad n \\ 3\Big[2(n+2)+\sum\limits_{k=n/2+2}^{n+1} 4(2k-1)+\sum\limits_{k=n/2+2}^{n+1} 4(2k)\Big]+ \\ 1\Big[\sum\limits_{k=n/2+2}^{n+1} 4(2k)+4(2n+3)\Big], \text{even} \quad n. \end{cases}$$



*[5]*phenacene: picene
(five rings)

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}. In G, 4 vertices



*[6]*phenacene: fulminene

(six rings)

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:

TEP$(C^*_{4\times 5+2}, x) = 4x^6 + 6x^7 + 6x^8 + 6x^9 + 6x^{10} + 2x^{11}$
TEP$(C^*_{4\times 6+2}, x) = 4x^7 + 6x^8 + 6x^9 + 6x^{10} + 6x^{11} + 6x^{12} + 2x^{13}$
TEP$(C^*_{4\times 7+2}, x) = 4x^8 + 6x^9 + 6x^{10} + 6x^{11} + 6x^{12} + 6x^{13} + 6x^{14} + 2x^{15}$

and thus,

TEP$(C^*_{4n+2}, x) = 4x^{n+2} + \sum_{k=n+3}^{2n+2} 6x^k + 2x^{2n+3}$

and

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

$$\prod E_1(C^*_{4n+2}) = [(n+2)^2]^4 \Big[\sum_{k=n+3}^{2n+2} [(k)^2]^6 \Big] \Big[(2n+3)^2 \Big]^2, n \geq 4\,,$$

and the eccentricity connectivity index is

$$\xi(C^*_{4n+2})\,.$$

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