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On Neighborhood Eccentricities Indices of Graphs

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Abstract

The topological indices are useful tools to the theoretical chemists that are provided by graph theory. They correlate certain physicochemical properties such as boiling point, strain energy, stability, etc. of chemical compounds. In this paper, we consider new graph invariants, based on the eccentricities of all the neighbors of a vertex in a graph, and so-called the neighborhood eccentricities indices. The neighborhood eccentricities indices of some chemical graph is calculated.

Key words: Eccentricity; N_e-degree (of vertex); N_e-indices; Topological Indices

2010 Mathematics Subject Classification : 05C07, 05C90

1 Introduction

Throughout this paper, we consider the connected, undirected simple graph. The basic definitions and concepts used in this study are adopted from [1, 9].

Given a graph $G = (V(G), E(G))$, the cardinality $|V(G)| = n$ of the vertex set $V(G)$ is the order of G. The neighborhood of a vertex $v \in V(G)$ is defined as the set $N(v)$ consisting of all vertices u which are adjacent with v.The degree of a vertex v in a graph G denoted by $deg(v)$ is the number of its neighbors, that is, $deg(v) = |N(v)|$. The distance $d(u, v)$ between any two vertices u and v of G is the length of the shortest path (number of edges) joining them. The eccentricity of a vertex v, denoted $e(v)$, in a graph G, is the

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distance between v and a vertex farthest from v, that is, $e(v) = max\{d(v, u) : u \in V(G)\}$.

The topological indices are the useful tools to the theoretical chemists that are provided by graph theory. A topological index is a real number related to a graph. These are graph invariants. In mathematical chemistry, these are known as molecular descriptors. Topological indices are the mathematical measures which correlate to the structures of any simple finite graphs. It does not depend on the labeling or the pictorial representation of a graph. The vertices and edges of molecular graphs correspond to the atoms of the compounds and chemical bonds, respectively. Topological indices play a vital role in mathematical chemistry specially, in chemical documentation, isomer discrimination and correlate certain physicochemical properties such as boiling point, strain energy and stability etc. of chemical compounds. It studies Quantitative structure activity (QSAR) and structure property (QSPR) relationships that are used to predict the biological activities and properties of the chemical compounds.

The oldest molecular index is the one put forward in 1947 by Wiener [16], and defined as the sum of distance between all pairs of vertices of a graph G, that is

$$W = \sum_{i<j} d(v_i, v_j).$$

The first and second Zagreb indices have been introduced by Gutman and Trinajesti [8], and are defined as:

$$M_1(G) = \sum_{u \in V(G)} deg(u)^2$$

$$M_2(G) = \sum_{uv \in E(G)} deg(u)deg(v).$$

In an analogy with the first and the second Zagreb indices, M. Ghorbani et al. and D. Vukicevic et al. define the first E_1, and the second E_2, Zagreb eccentricity indices by [4, 15]

$$E_1(G) = \sum_{v \in V(G)} e(v)^2$$

$$E_2(G) = \sum_{uv \in E(G)} e(u)e(v).$$

The total eccentricity of the graph G [2, 14], denoted by $\xi(G)$, is defined as the sum of eccentricities of all vertices of graph G, that is

$$\xi(G) = \sum_{v \in V(G)} e(v).$$

Sharma, Goswami and Madan [13] introduced the eccentric connectivity index and which they defined as

$$\xi^c(G) = \sum_{v \in V(G)} deg(v)e(v).$$

For further study and literature related to the eccentric topological indices, see references [6, 10, 12, 17].
In [5], Graovac et al. defined the fifth M-Zagreb indices as

$$M_1G_5(G) = \sum_{uv \in E(G)} (S(u) + S(v))$$

$$M_2G_5(G) = \sum_{uv \in E(G)} S(u)S(v).$$

Where $S(v) = \sum_{u \in N(v)} deg(u)$.

A new version of Zagreb index called fifth M_3-Zagreb index is defined by Kulli in [11],

$$M_3G_5(G) = \sum_{uv \in E(G)} |S(u) - S(v)|.$$

In literature, mathematical chemists used combinations of vertex degree, edge degree, vertex eccentricity, open neighbourhood degree sum, etc., to define several topological indices and to study their applications in chemistry. Recently, S. Ediz [3], in 2017, introduced S-indices of connected graphs, throughout of them the first S-index of G defined as;

$$S_1(G) = \sum_{v \in V(G)} s(v)^2,$$

where $s(v) = |M_v - S_v|, S_v = \sum_{u \in N(v)} deg(u)$ and $M_v = \prod_{u \in N(v)} deg(u)$.

In this paper, motivated by the S-indices of graphs, we investigate the effect of the eccentricities of the neighbours vertices along with the vertex itself, we proceed to introduce new version of topological indices of a connected graph G based on the eccentricities sum and the eccentricities product of the open neighbourhood of a vertex in a graph, and so-called them the first, second and third neighborhood eccentricities indices (in short N_e-indices) of a graph G and denoted them by $N_e^1(G)$, $N_e^2(G)$ and $N_e^3(G)$, respectively. The exact formulas of $N_e^1(G)$ for some chemical graphs is computed.

2 N_e-degrees and N_e-indices of a graph

For a vertex $v \in V(G)$, the open neighborhood of v in G, denoted $N(v)$, is the set of all vertices that are adjacent to v. For a vertex v, $T_v = \sum_{u \in N(v)} e(u)$, and $W_v = \prod_{u \in N(v)} e(u)$. The N_e-degree of a vertex v of a connected graph G defined as

$$d_{ne}(v) = |W_v - T_v|.$$

Lemma 2.1. For a nontrivial connected graph G and a vertex $v \in V(G)$,

1. If $deg(v) = 1$, then $d_{ne}(v) = 0$.
2. If $deg(v) = 2$, then $d_{ne}(v) = 0$, if and only if $e(u) = 2$, for every $u \in N(v)$.

Definition 2.2. The first, second and third neighborhood eccentricities indices of a graph G are defined as

$$N_e^1(G) = \sum_{v \in V(G)} d_{ne}(v).$$

$$N_e^2(G) = \sum_{uv \in E(G)} d_{ne}(u)d_{ne}(v).$$

$$N_e^3(G) = \sum_{uv \in E(G)} d_{ne}(u) + d_{ne}(v).$$

3 N_e^1-indix of cycloalkenes

We denote a cycloalkene having n carbon atoms and $2n-2$ hydrogen atoms by C_n^{2n-2}. The molecular graphs of them are obtained by attaching $2n-2$ pendant vertices corresponding to hydrogen atoms to vertices of a cycle corresponding to carbon atoms as shown in Figure 1.

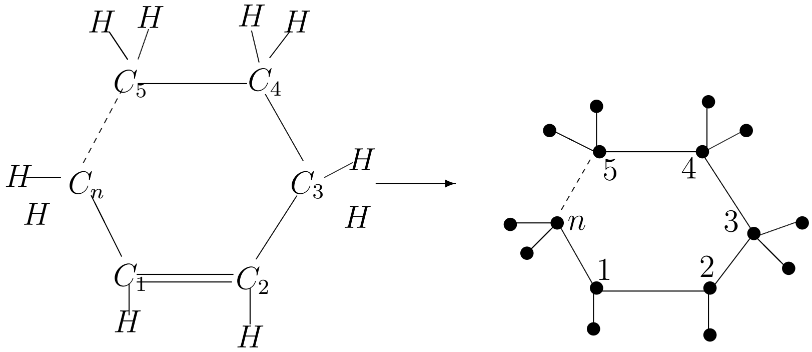

Figure 1: A cycloalkene and its graph model

Theorem 3.1. For $n \geq 3$, the first T index of a cycloalkene molecular graph is given by

$$N_e^1(C_n^{2n-2}) = \begin{cases} \frac{n^5}{16} + \frac{5n^4}{8} + 2n^3 - \frac{n^2}{2} - 8n, \text{ if } n \text{ is even ;} \\ \\ \frac{n^5}{16} + \frac{7n^4}{8} + 2n^3 - \frac{5n^2}{2} - \frac{57n}{8} + \frac{21}{8}, \text{ if } n \text{ is odd.} \end{cases}$$

Proof: The cycloalkene molecular graph C_n^{2n-2} has $3n-2$ vertices including two vertices (namely, C_1 and C_2) of degree three, $n-2$ vertices $C_3, C_4, ..., C_n$ of degree four and correspond to the carbon atoms of cycloalkenes and the remaining $2n-2$ vertices (namely, $H's$) are end vertices with and they correspond to hydrogen atoms of cycloalkenes. Thus we have the following cases:

Case 1: If n is even, then $e(C_i) = \frac{n}{2} + 1$, for $1 \leq i \leq n$ and $e(H) = \frac{n}{2} + 2$.
Since, $deg(H) = 1$. Then by Lemma 2.1, $d_{ne}(H) = |W_H - T_H| = 0$, for every $H \in V(C_n^{2n-2})$.
The vertices C_1 and C_2 of carbon atoms has 3 neighborhood vertices, that two vertices of carbon atoms and one vertex of hydrogen, so for $i = 1, 2$

$$\begin{aligned} T_{C_1} = T_{C_2} &= \frac{n}{2} + 1 + \frac{n}{2} + 1 + \frac{n}{2} + 2 \\ &= \frac{3n}{2} + 4, \end{aligned}$$

$$\begin{aligned} W_{C_1} = W_{C_2} &= (\frac{n}{2} + 1)(\frac{n}{2} + 1)(\frac{n}{2} + 2) \\ &= \frac{n^3}{8} + n^2 + \frac{5n}{2} + 2. \end{aligned}$$

Hence,

$$\begin{aligned} d_{ne}(C_1) = d_{ne}(C_2) &= |W_{C_1} - T_{C_1}| \\ &= |\frac{n^3}{8} + n^2 + \frac{5n}{2} + 2 - \frac{3n}{2} - 4| \\ &= \frac{n^3}{8} + n^2 + n - 2. \end{aligned} \tag{1}$$

Since every vertex C_i, for $3 \leq i \leq n$ of carbon atoms has four neighbors, that two vertices of carbon atoms and two vertices of hydrogen, so for $3 \leq i \leq n$,

$$\begin{aligned} T_{C_i} &= \frac{n}{2} + 1 + \frac{n}{2} + 1 + \frac{n}{2} + 2 + \frac{n}{2} + 2 \\ &= 2n + 6, \end{aligned}$$

$$\begin{aligned} W_{C_i} &= (\frac{n}{2} + 1)(\frac{n}{2} + 1)(\frac{n}{2} + 2)(\frac{n}{2} + 2) \\ &= \frac{n^4}{16} + n^2 + \frac{3n^3}{4} + \frac{13n^2}{4} + 6n + 4. \end{aligned}$$

Then,

$$\begin{aligned} d_{ne}(C_i) &= |W_{C_i} - T_{C_i}| \\ &= \frac{n^4}{16} + n^2 + \frac{3n^3}{4} + \frac{13n^2}{4} + 4n - 2. \end{aligned} \tag{2}$$

By collecting $d_{ne}(H)$ and $d_{ne}(C_i)$, for $1 \leq i \leq n$, from Equations 1 and 2, we get the following result

$$\begin{aligned} N_e^1(C_n^{2n-2}) &= \sum_{v \in V(C_n^{2n-2})} d_{ne}(v) \\ &= \sum_{i=1}^{2n-2} d_{ne}(H_i) + \sum_{i=1}^{n} d_{ne}(C_i) \\ &= (2n-2)d_{ne}(H) + 2d_{ne}(C_1) + \sum_{i=3}^{n} d_{ne}(C_i) \\ &= 0 + 2(\frac{n^3}{8} + n^2 + n - 2) + (n-2)(\frac{n^4}{16} + n^2 + \frac{3n^3}{4} + \frac{13n^2}{4} + 4n - 2) \\ &= \frac{n^3}{4} + 2n^2 + 2n - 4 + \frac{n^5}{16} + \frac{5n^4}{8} + \frac{7n^3}{4} - \frac{5n^2}{2} - 10n + 4. \\ &= \frac{n^5}{16} + \frac{5n^4}{8} + 2n^3 - \frac{n^2}{2} - 8n. \end{aligned}$$

Case 2: If n is odd, then for $1 \leq i \leq n$, $e(C_i) = \frac{n-1}{2} + 1$ and $e(H) = \frac{n-1}{2} + 2$. By Lemma 2.1, $d_{ne}(H) = 0$ for all hydrogen atoms. Since, the vertices C_1 and C_2 of carbon atoms has 3 neighborhood vertices, that two vertices of carbon atoms and one vertex of hydrogen . Hence, for $i = 1, 2$

$$\begin{aligned}
T_{C_1} = T_{C_2} &= \frac{n-1}{2} + 2 + \frac{n-1}{2} + 1 + \frac{n-1}{2} + 1 \\
&= \frac{3(n-1)}{2} + 4, \\
W_{C_1} = W_{C_2} &= (\frac{n-1}{2} + 2)(\frac{n-1}{2} + 1)(\frac{n-1}{2} + 1) \\
&= \frac{n^3 + 5n^2 + 7n + 3}{8}.
\end{aligned}$$

and

$$\begin{aligned}
d_{ne}(C_1) = d_{ne}(C_2) &= |W_{C_1} - T_{C_2}| \\
&= |\frac{n^3 + 5n^2 + 7n + 3}{8} - (\frac{3(n-1)}{2} + 4)| \\
&= \frac{n^3 + 5n^2 - 5n - 17}{8}. \qquad (3)
\end{aligned}$$

Since every vertex C_i, $3 \leq i \leq n$ of carbon atoms has 4 neighborhood vertices, that two vertices of carbon atoms and two vertices of hydrogen, so

$$\begin{aligned}
T_{C_i} &= \frac{n-1}{2} + 1 + \frac{n-1}{2} + 1 + \frac{n-1}{2} + 2 + \frac{n-1}{2} + 2 \\
&= 2n + 4,
\end{aligned}$$

$$\begin{aligned}
W_{C_i} &= (\frac{n-1}{2} + 1)(\frac{n-1}{2} + 1)(\frac{n-1}{2} + 2)(\frac{n-1}{2} + 2) \\
&= \frac{n^4}{16} + \frac{n^3}{2} + \frac{11n^2}{8} + \frac{3n}{2} + \frac{9}{16}.
\end{aligned}$$

Then,

$$\begin{aligned}
d_{ne}(C_i) &= |W_{C_i} - T_{C_i}| \\
&= |\frac{n^4}{16} + \frac{n^3}{2} + \frac{11n^2}{8} + \frac{3n}{2} + \frac{9}{16} - 2n - 4| \\
&= \frac{n^4}{16} + \frac{n^3}{2} + \frac{11n^2}{8} - \frac{n}{2} - \frac{55}{16}. \qquad (4)
\end{aligned}$$

By collecting $d_{ne}(H)$ and $d_{ne}(C_i)$, for $i = 1, 2, ..., n$, from Equations (3) and (4), we get the following result

$$\begin{aligned}
N_e^1(C_n^{2n-2}) &= \sum_{v\in V(C_n^{2n-2})} d_{ne}(v) \\
&= \sum_{i=1}^{2n-2} d_{ne}(H_i) + \sum_{i=1}^{n} d_{ne}(C_i) \\
&= (2n-2)d_{ne}(H) + 2d_{ne}(C_1) + \sum_{i=3}^{n} d_{ne}(C_i) \\
&= 0 + 2(\frac{n^3+5n^2-5n-17}{8}) + (n-2)(\frac{n^4}{16} + \frac{n^3}{2} + \frac{11n^2}{8} - \frac{n}{2} - \frac{55}{16}) \\
&= \frac{n^3+5n^2-5n-17}{4} + \frac{n^5}{16} + \frac{7n^4}{8} + \frac{7n^3}{4} - \frac{15n^2}{4} - \frac{47}{8}n + \frac{55}{8}. \\
&= \frac{n^5}{16} + \frac{7n^4}{8} + \frac{7n^3}{4} - \frac{15n^2}{4} - \frac{47}{8}n + \frac{55}{8} \\
&= \frac{n^5}{16} + \frac{7n^4}{8} + 2n^3 - \frac{5n^2}{2} - \frac{57n}{8} + \frac{21}{8}.
\end{aligned}$$

■

4 N_e^1-index of Alkanes

In this section, we construct the general formulas for the N_e^1-index of a chemical trees which represent of an alkane compound. Alkanes are hydrocarbons with only single bonds between the atoms, and it has a general formula P_nH_{2n+2}, where n is number of carbon atoms.

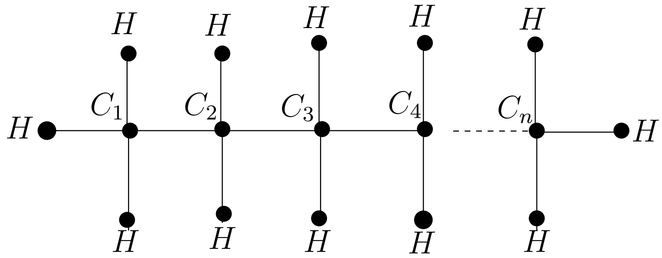

Figure 2: Clsses of alkanes C_nH_{2n+2}

Theorem 4.1. For $n \geq 7$, the first N_e^1 index of alkanes graph C_nH_{2n+2} is given by

$$N_e^1(C_nH_{2n+2}) = \begin{cases} \frac{31n^5}{80} + \frac{15n^4}{8} + \frac{n^3}{48} + \frac{13n^2}{4} - \frac{n}{30} + 14, \text{ if } n \text{ is even;} \\ \\ \frac{31n^5}{80} + \frac{45n^4}{16} + \frac{79n^3}{12} + \frac{69n^2}{8} - \frac{72n}{15} + \frac{81}{16}, \text{ if } n \text{ is odd.} \end{cases}$$

Proof: The alkene molecular graph C_nH_{2n+2}, $n \geq 7$, has $3n+2$ vertices including n vertices $C_1, C_2, ..., C_n$ of degree four and correspond to the carbon atoms of alkenes and the remaining $2n+2$ vertices (namely, H's) are end vertices with degree one and they correspond to hydrogen atoms of alkenes. Since, the eccentricity vertex set of alkenes is a symmetric around the center vertex set and $e(v_i) = e(v_{n+1-i})$, for every $i = 1, 2, ..., n$ and every $v_i \in V(C_nH_{2n+2})$.
Since, for every $H \in V(C_nH_{2n+2})$, $deg(H) = 1$. Then by Lemma 2.1,

$$d_{ne}(H) = |W_H - T_H| = 0.$$

Thus we have the following two cases:

Case 1: n is even, It is clear that, the center set of C_nH_{2n+} is $\{C_{\frac{n}{2}}, C_{\frac{n}{2}+1}\}$ and hence every C_i, $i = 1, 2, ..., \frac{n}{2} - 1$ has three neighbors with $e = n + 2 - i$ and one neighbor with eccentricity $e = n - i$, whereas $C_{\frac{n}{2}}$ has three neighbors with $e = .\frac{n}{2} + 2$ and one with $e = \frac{n}{2} + 1$. Thus

$$T_{C_i} = T_{C_{n+1-i}} = 3(n+2-i) + (n-i) = 4(n-i) + 6.$$

$$W_{C_i} = W_{C_{n+1-i}} = (n+2-i)^3(n-i) = (n-i)^4 + 6(n-i)^3 + 12(n-i)^2 + 8(n-i).$$

Hence,

$$d_{ne}(C_i) = d_{ne}(C_{n+1-i}) = |W_{C_i} - T_{C_i}| = (n-i)^4 + 6(n-i)^3 + 12(n-i)^2 + 4(n-i) - 6.$$

For the central vertex, we get

$$T_{C_{\frac{n}{2}}} = T_{C_{\frac{n}{2}+1}} = 3(\frac{n}{2} + 2) + (\frac{n}{2} + 1) = 2n + 7$$

$$W_{C_{\frac{n}{2}}} = W_{C_{\frac{n}{2}+1}} = (\frac{n}{2} + 2)^3(\frac{n}{2} + 1) = \frac{1}{16}(n^4 + 14n^3 + 72n^2 + 160n + 128)$$

and hence, $d_{ne}(C_{\frac{n}{2}}) = d_{ne}(C_{\frac{n}{2}+1}) = \frac{1}{16}(n^4 + 14n^3 + 72n^2 + 128n + 16)$.

Therefore,

$$\begin{aligned}
N_e^1(C_nH_{2n+2}) &= 2\Big[d_{ne}(C_{\frac{n}{2}}) + \sum_{i=1}^{\frac{n}{2}-1} d_{ne}(C_i)\Big] \\
&= \frac{1}{8}(n^4+14n^3+72n^2+128n+16) \\
&+ 2\sum_{i=1}^{\frac{n}{2}-1}\Big[(n-i)^4+6(n-i)^3+12(n-i)^2+4(n-i)-6\Big] \\
&= \frac{1}{8}(n^4+14n^3+72n^2+128n+16) + 2\sum_{i=1}^{\frac{n}{2}-1}(n^4+6n^3+12n^2+4n-6) \\
&- 2(4n^3+18n^2+24n-12)\sum_{i=1}^{\frac{n}{2}-1} i + 2(6n^2+18n+12)\sum_{i=1}^{\frac{n}{2}-1} i^2 \\
&- 2(4n+6)\sum_{i=1}^{\frac{n}{2}-1} i^3 + 2\sum_{i=1}^{\frac{n}{2}-1} i^4.
\end{aligned}$$

By take the values of the summations and simple computing, we get

$$\begin{aligned}
N_e^1(C_nH_{2n+2}) &= \frac{1}{8}(n^4+14n^3+72n^2+128n+16) + 2(\frac{n}{2}-1)(n^4+6n^3+12n^2+4n-6) \\
&- (4n^3+18n^2+24n-12)(\frac{n^2-2n}{4}) + (6n^2+18n+12)(\frac{n^3-3n^2+2n}{12}) \\
&- (4n+6)(\frac{n^4-4n^3+4n^2}{32}) + \frac{3n^5-15n^4+20n^3-8n}{240} \\
&= \frac{31n^5}{80} + \frac{15n^4}{8} + \frac{n^3}{48} + \frac{13n^2}{4} - \frac{n}{30} + 14.
\end{aligned}$$

Case 2: n is odd, the center set of C_nH_{2n+} is $\{C_{\frac{n+1}{2}}\}$ and hence every C_i, $i = 1, 2, ..., \frac{n-1}{2}$ has three neighbors with $e = n+2-i$ and one neighbor with eccentricity $e = n-i$, whereas $C_{\frac{n+1}{2}}$ has four neighbors with $e = .\frac{n+3}{2}$. Thus, for $1 \leq i \leq \frac{n-1}{2}$,

$$T_{C_i} = T_{C_{n+1-i}} = 3(n+2-i) + (n-i) = 4(n-i) + 6.$$

$$W_{C_i} = W_{C_{n+1-i}} = (n+2-i)^3(n-i) = (n-i)^4 + 6(n-i)^3 + 12(n-i)^2 + 8(n-i).$$

Hence,

$$d_{ne}(C_i) = d_{ne}(C_{n+1-i}) = |W_{C_i} - T_{C_i}| = (n-i)^4 + 6(n-i)^3 + 12(n-i)^2 + 4(n-i) - 6.$$

For the central vertex, we get

$$T_{C_{\frac{n+1}{2}}} = 2n + 6$$

$$W_{C_{\frac{n+1}{2}}} = (\frac{n+3}{2})^4$$

and hence, $d_{ne}(C_{\frac{n+1}{2}}) = \frac{1}{16}(n^4 + 12n^3 + 54n^2 + 76n - 15)$.
Therefore,

$$\begin{aligned}
N_e^1(C_nH_{2n+2}) &= d_{ne}(C_{\frac{n+1}{2}}) + 2\sum_{i=1}^{\frac{n-1}{2}} d_{ne}(C_i) \\
&= \frac{1}{16}(n^4 + 12n^3 + 54n^2 + 76n - 15) \\
&+ 2\sum_{i=1}^{\frac{n+1}{2}} \Big((n-i)^4 + 6(n-i)^3 + 12(n-i)^2 + 4(n-i) - 6\Big) \\
&= \frac{1}{16}(n^4 + 12n^3 + 54n^2 + 76n - 15) + 2\sum_{i=1}^{\frac{n-1}{2}}(n^4 + 6n^3 + 12n^2 + 4n - 6) \\
&- 2(4n^3 + 18n^2 + 24n - 12)\sum_{i=1}^{\frac{n-1}{2}} i + 2(6n^2 + 18n + 12)\sum_{i=1}^{\frac{n-1}{2}} i^2 \\
&- 2(4n + 6)\sum_{i=1}^{\frac{n-1}{2}} i^3 + 2\sum_{i=1}^{\frac{n-1}{2}} i^4
\end{aligned}$$

$$\begin{aligned}
N_e^1(C_nH_{2n+2}) &= \frac{1}{16}(n^4 + 12n^3 + 54n^2 + 76n - 15) + (n-1)(n^4 + 6n^3 + 12n^2 + 4n - 6) \\
&- (4n^3 + 18n^2 + 24n + 4)(\frac{n(n-2)}{4}) + (6n^2 + 18n + 12)(\frac{n^3 - 3n^2 + 2n}{12}) \\
&- (4n + 6)(\frac{n^4 - 4n^3 + 4n^2}{32}) + (\frac{3n^5 - 15n^4 + 20n^3 - 8n}{240}) \\
&= \frac{31n^5}{80} + \frac{45n^4}{16} + \frac{79n^3}{12} + \frac{69n^2}{8} - \frac{72n}{15} + \frac{81}{16}.
\end{aligned}$$

∎

5 N_e^1 index of $C_n^{R_r}$

In this section, we construct general formula for N_e^1-index of the chemical graph cycloalkyls that is constructed by attaching an alkyl R_r instead of each hydrogen atoms in the cycloalkenes.

We denote the group of alkyls by $R_r, r \in \mathbb{Z}^+$. For example $R_1, R_2, R_3, ...$ denote methyl,

ethyl, propyl,..., respectively, as shown in Figure 3.
When we put an alkyl instead of each hydrogen atom in the cycloalkene, we get a cycloalkyls and denoted by $C_n^{R_r}$ as shown in Figure 4.

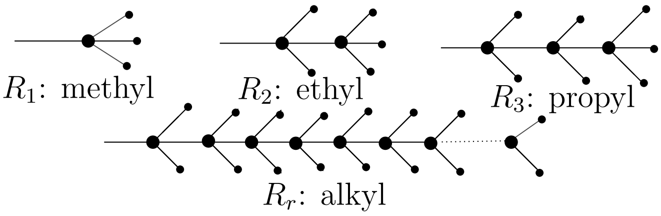

Figure 3: The first few alkyls

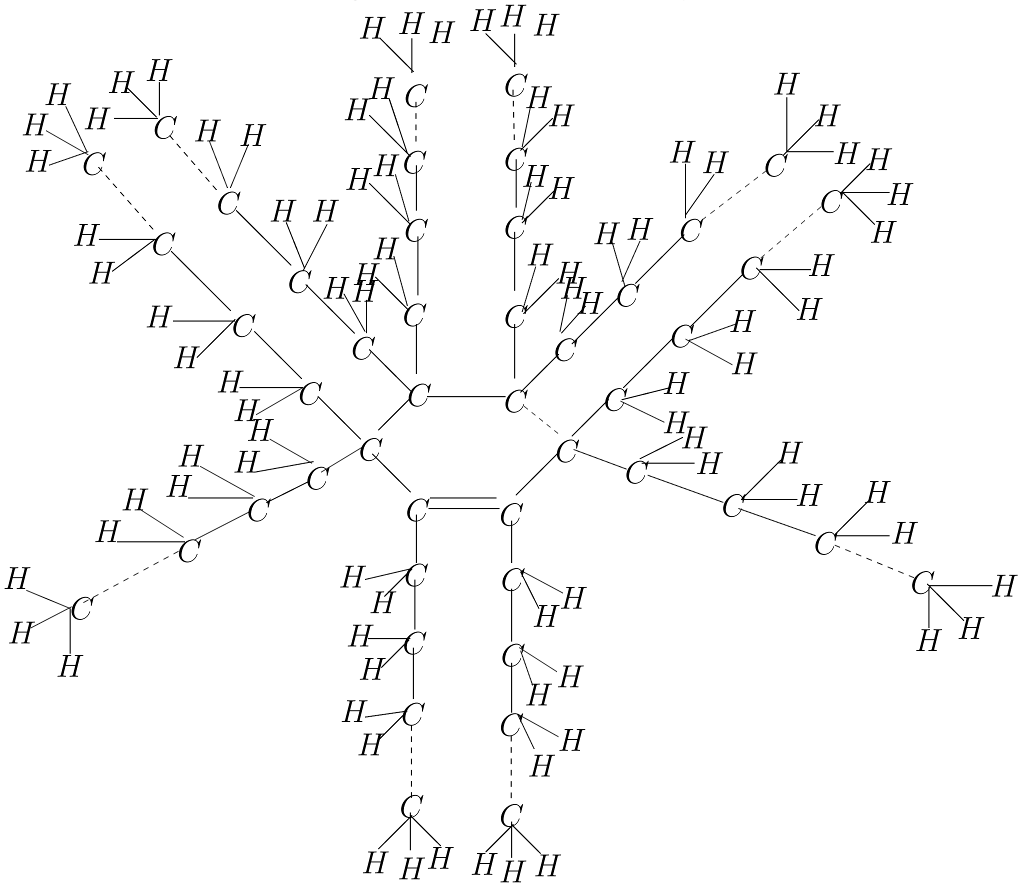

Figure 4: Molecular structure of $C_n^{R_r}$

Theorem 5.1. For positive integers $n \geq 3$ and $r \geq 1$, the frist N_e^1-index farmula of the cycloalkyls graph is given by

$$N_e^1(C_n^{R_r}) = [(n-2) + 2r(n-1)]\Big(\lfloor\frac{n}{2}\rfloor + r\Big)^4 + [(6n-10) + 4r(n-1)(r+4)]\Big(\lfloor\frac{n}{2}\rfloor + r\Big)^3$$

$$+ [(13n-18) + 8r(n-1)(r^2+6r+8)]\Big(\lfloor\frac{n}{2}\rfloor + r\Big)^2$$
$$+ [(n-12) + 2r(n-1)(r^3+8r^2+2r+19)]\Big(\lfloor\frac{n}{2}\rfloor + r\Big)$$
$$- [2n + r(n-1)(\frac{6r^4+60r^3+220r^2+285r+299}{15})].$$

Where $\lfloor\frac{n}{2}\rfloor = \begin{cases} \frac{n}{2}, & \text{if } n \text{ even;} \\ \frac{n-1}{2}, & \text{if } n \text{ odd.} \end{cases}$.

Proof: For positive integers $n \geq 3$ and $r \geq 1$, the vertex set of the cycloalkyls molecular graph $C_n^{R_r}$ can be divided into three kinds of vertices. Kind 1, the vertices on the cycle, denoted by $\{C_i : 1 \leq i \leq n\}$, correspond to the carbon atoms of cycloalkenes, tow of them (namely, C_1 and C_2) of degree three and $n-2$ vertices $C_3, C_4, ..., C_n$ of degree four. Kind 2, the vertices on the path, denoted by $\{C_j^{(ik)} : 1 \leq j \leq r,\ \ 1 \leq i \leq n\ \ and\ \ k = 1, 2\}$, correspond to the carbon atoms of alkenes, branches, all of them with degree four. Kind 3, the remaining vertices (namely, $H's$) are end vertices with degree one and they correspond to hydrogen atoms of cycloalkyls. By easy chick, for any $n \geq 3$, we get $e(C_i) = \lfloor\frac{n}{2}\rfloor + r + 1$, $e(C_j^{(ik)}) = \lfloor\frac{n}{2}\rfloor + r + j + 1$ and $e(H^{(j)}) = e(C_j^{(ik)}) + 1$, for $1 \leq i \leq n$, $1 \leq j \leq r$ and $k = 1, 2$. Hence, for every $H \in V(C_n^{R_r})$, correspond to hydrogen atoms, $deg(H) = 1$. Then by Lemma 2.1, $d_{ne}(H) = |W_H - T_H| = 0$.
In the next, we put $X = \lfloor\frac{n}{2}\rfloor + r$, to easy compute.
The vertices C_1 and C_2 of carbon atoms on cycle has three neighborhood vertices, that two vertices of carbon atoms and one vertex of alkyl, so for $i = 1, 2$

$$T_{C_1} = T_{C_2} = 2(X+1) + (X+2) = 3X + 4,$$
$$W_{C_1} = W_{C_2} = (X+1)^2(X+2) = X^3 + 4X^2 + 5X + 2$$

thus, $d_{ne}(C_1) = d_{ne}(C_2) = |W_{C_1} - T_{C_1}| = X^3 + 4X^2 + 2X - 2.$ (1)

For $3 \leq i \leq n$

$$T_{C_i} = 2(X+1) + 2(X+2) = 4X + 6,$$
$$W_{C_1} = W_{C_2} = (X+1)^2(X+2)^2 = X^4 + 6X^3 + 13X^2 + 12X + 4,$$

thus, $d_{ne}(C_i) = |W_{C_i} - T_{C_i}| = X^4 + 6X^3 + 13X^2 + 8X - 2.$ (2)

For $1 \leq j \leq r$, $1 \leq i \leq n$ and $k = 1, 2$,

$$T_{C_j^{(ik)}} = 3(X + j + 2) + (X + j) = 4X + 4j + 2,$$

$$\begin{aligned} W_{C_j^{(ik)}} &= (X + j + 2)^3(X + j) = [X^3 + 3X^2(j + 2) + 3X(j + 2)^2 + (j + 2)^3][X + j] \\ &= (X^4 + 6X^3 + 12X^2 + 8X) + (4X^3 + 18X^2 + 24X + 8)j \\ &+ (6X^2 + 18X + 12)j^2 + (4X + 6)j^3 + j^4, \end{aligned}$$

Hence,

$$\begin{aligned} d_{ne}(C_j^{(ik)}) &= |W_{C_j^{(ik)}} - T_{C_j^{(ik)}}| \\ &= (X^4 + 6X^3 + 12X^2 + 4X - 6) + (4X^3 + 18X^2 + 24X + 4)j \\ &+ (6X^2 + 18X + 12)j^2 + (4X + 6)j^3 + j^4. \end{aligned} \tag{3}$$

Therefore, from (1), (2) and (3), we get

$$\begin{aligned} N_e^1(C_n^{R_r}) &= 2d_{ne}(C_1) + \sum_{i=}^{n} d_{ne}(C_i) + (2n - 2)\sum_{j=1}^{r} d_{ne}(C_j^{(ik)}) \\ &= 2(X^3 + 4x^2 + 2X - 2) + (n - 2)(X^4 + 6X^3 + 13x^2 + 8X - 2) \\ &+ (2n - 2)\sum_{j=1}^{r}\Big[(X^4 + 6X^3 + 12X^2 + 4X - 6) + (4X^3 + 18X^2 + 24X + 4)j \\ &+ (6X^2 + 18X + 12)j^2 + (4X + 6)j^3 + j^4\Big] \end{aligned}$$

$$\begin{aligned} N_e^1(C_n^{R_r}) &= [(n - 2)X^4 + (6n - 10)X^3 + (13n - 18)X^2 + (n - 12)X - 2n] \\ &+ (2n - 2)\Big[r(X^4 + 6X^3 + 12X^2 + 4X - 6) + (4X^3 + 18X^2 + 24X + 4)\sum_{j=1}^{r} j\Big] \\ &+ (2n - 2)\Big[(6X^2 + 18X + 12)\sum_{j=1}^{r} j^2 + (4X + 6)\sum_{j=1}^{r} j^3 + \sum_{j=1}^{r} j^4\Big] \\ &= [(n - 2 + 2r(n - 1))X^4 + (6n - 10 + 12r(n - 1))X^3 + (13n - 18 + 24r(n - 1))X^2 \\ &+ (n - 12 + 8r(n - 1))X - 2n - 12(n - 1)] \\ &+ (2n - 2)\Big[(4X^3 + 18X^2 + 24X + 4)(\frac{r(r + 1)}{2}) + (6X^2 + 18X + 12)(\frac{r(r + 1)(2r + 1)}{6} \\ &+ (2n - 2)\Big[(4X + 6)(\frac{r^2(r + 1)^2}{4}) + (\frac{r(r + 1)(2r + 1)(3r^2 + 3r - 1)}{30})\Big] \end{aligned}$$

$$
\begin{aligned}
&= [(n-2)+2r(n-1)]X^4 + [(6n-10)+4r(n-1)(r+4)]X^3 \\
&+ [(13n-18)+8r(n-1)(r^2+6r+8)]X^2 + [(n-12) \\
&+ 2r(n-1)(r^3+8r^2+2r+19)]X \\
&- [2n+r(n-1)(\frac{6r^4+60r^3+220r^2+285r+299}{15})].
\end{aligned}
$$

■

6 Conclusion

In this paper, we studied the effect of the eccentricities of the neighbours vertices along with the vertex itself. The neighborhood eccentricity degree of a vertex v in a graph G is defined and denoted by $d_{ne}(v)$. Furthermore, we introduced three new versions of the topological indices of a connected graphs based on the eccentricities sum and the eccentricities product of the open neighbourhood of a every vertex in a graph G, and are called the first, second and third neighborhood eccentricities indices and denoted by $N_e^1(G)$, $N_e^2(G)$ and $N_e^3(G)$, respectively. The exact formulas of $N_e^1(G)$ for some chemical graphs is computed.

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