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Some topological indices of certain classes of cycloalkenes

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Abstract

Let $G = (V, E)$ be a simple connected molecular graph. The degree d_i of any vertex v_i in G is the number of edges incident with v_i and the eccentricity e_i of v_i is the largest distance between v_i and any other vertex of G. In this paper, we establish general formulae for some degree based and eccentricity based topological indices of cycloalkenes.

Keywords: degree, eccentricity, Zagreb index, molecular graph, alkyl, cycloalkenes

MSC Numbers: 05C07, 05C30, 05C90

1 Significance of the work

Chemical applications of graph theory are increasingly in use nowadays and there are many papers aiming these applications. Most of these applications depends on the fact that every chemical molecule can be modelled by a graph called a molecular or chemical graph and studying mathematical properties of this model graph helps one to estimate some physico-chemical properties of the corresponding molecule. There are many topological graph indices defined for this aim. The cycloalkenes are unsaturated hydrocarbons having a few hydrogen atoms and only a few bonds. Unlike open chain alkenes, cycloalkenes have less hydrogen atoms and less bonds. So, there is less intermolecular energy within the molecule. In this paper, we establish the general formulae for the first and second Zagreb indices, first and second Zagreb eccentricity indices and first and second Zagreb degree eccentricity indices of molecular graph of cycloalkenes.

2 Introduction

Chemical graph theory is one of the well-investigated application areas with several researchers working on applications of graph theory to discover some chemical phenomena by means of mathematical modelling. If we represent the atoms of a molecule by vertices and the chemical covalent bonds between the atoms by edges, the graph obtained is a mathematical model of the given molecule. Such graphs usually referred as molecular graphs or chemical graphs. They clearly give a graph-theoretical representation of the molecule under consideration and provide valuable information on the required chemical phenomena, [1].

Cycloalkenes are unsaturated hydrocarbons having a few hydrogen atoms and a few bonds. Unlike open chain alkenes, cycloalkenes have less hydrogen atoms and less bonds. So, there is less intermolecular energy within the molecule. The important properties of cycloalkenes are as follows: at room temperature most of them are in liquid state inspite of having very low solubility in water. But the first few cycloalkenes are in gaseous state and are rarely solid in room temperature. The cycloalkenes exhibit similar physical properties as cycloalkanes but differ in the fact that cycloalkenes have at least one double bond, [7].

Topological indices are numbers associated with chemical structures derived from their hydrogen-depleted graphs as a tool for compact and effective description of structural formulae which are used to study and predict the structure-property correlations of organic compounds. Molecular descriptors are playing significant role in Chemistry, Biology, Physics, Materials Science, Pharmacology, etc. In all these areas, topological indices have a prominent place, [11].

All the graphs $G = (V, E)$ considered in this paper are simple, undirected and connected graphs. For any vertices $u, v \in V(G)$, the distance $d(u, v)$ is defined as the length of the shortest path connecting u and v in G. For a vertex v_i in G, the degree d_i of v_i is the number of edges incident with v_i and in particular a vertex v_i in G is a pendant vertex if $d_i = 1$. The eccentricity e_i of v_i is the largest distance between v_i and any other vertex of G. The terminology used throughout this paper is based on [2].

An important topological index introduced more than fourty years ago by Gutman and Trinajstić is called the Zagreb index, [6]. For details and examples of chemical applications and mathematical theory of topological graph indices, see the surveys [4, 5, 8]. The first Zagreb index $M_1(G)$ of G is defined, [6], as

$$M_1(G) = \sum_{v_i \in V(G)} d_i^2$$

and the second Zagreb index $M_2(G)$ of G is defined as

$$M_2(G) = \sum_{v_i v_j \in E(G)} d_i d_j.$$

The invariants based on eccentricities attracted some attention in Chemistry. In analogy with the first and the second Zagreb indices, Ghorbani et al. and Vukičević et al. introduced the first and second Zagreb eccentricity indices, [3, 12], by replacing the vertex degrees with the eccentricities. The first Zagreb eccentricity E_1 and the second Zagreb eccentricity E_2 indices of a graph G are defined in [3] as

$$E_1(G) = \sum_{v_i \in V(G)} e_i^2$$

and

$$E_2(G) = \sum_{v_i v_j \in E(G)} e_i e_j.$$

The Zagreb degree eccentricity indices are introduced in [10]. First Zagreb degree eccentricity DE_1 and second zagreb degree eccentricity DE_2 indices of a graph G are defined as

$$DE_1 = \sum_{v_i \in V(G)} (e_i + d_i)^2$$

and

$$DE_2(G) = \sum_{v_i v_j \in E(G)} (e_i + d_i)(e_j + d_j).$$

Further studies on Zagreb degree eccentricity indices can be found in [9].

In this paper, we establish the general formulae for the first and second Zagreb indices, first and second Zagreb eccentricity indices and first and second Zagreb degree eccentricity indices of molecular graph of cycloalkenes.

3 Topological indices 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 Fig. 3.1.

Fig. 3.1 displays the molecular structure of cycloalkenes and the corresponding molecular graph of this cycloalkene as a chemical compound. We calculate some degree based and eccentricity based topological indices of the graph shown in Fig. 3.1 in what follows.

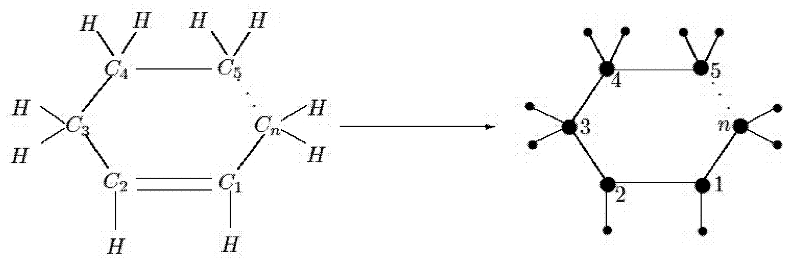

Figure 3.1 A cycloalkene and its graph model

Theorem 3.1. *Let $n \geq 3$ be a positive integer. Then the first and second Zagreb indices of the graph C_n^{2n-2} are*

$$M_1(C_n^{2n-2}) = 18n - 16$$

and

$$M_2(C_n^{2n-2}) = 24n - 25.$$

Proof. *Consider the graph C_n^{2n-2}, the molecular graph of a cycloalkene. It has $3n-2$ vertices. Out of these vertices, two vertices of degree 3 and $n-2$ vertices of degree 4 correspond to the carbon atoms of cycloalkenes. The remaining $2n-2$*

vertices are pendant vertices and they correspond to hydrogen atoms of cycloalkenes. Then

$$\begin{aligned}M_1(C_n^{2n-2}) =& \sum_{v_i \in V(C_n^{2n-2})} d_i^2\\ =&(n-2)\cdot 4^2 + 2\cdot 3^2 + (2n-2)\cdot 1^2\\ =&18n-16\end{aligned}$$

and

$$\begin{aligned}M_2(C_n^{2n-2}) =& \sum_{v_iv_j \in E(C_n^{2n-2})} d_id_j\\ =&(n-3)\cdot 4\cdot 4 + 2\cdot 4\cdot 3 + 1\cdot 3\cdot 3 + (2n-4)\cdot 1\cdot 4 + 2\cdot 1\cdot 3\\ =&24n-25.\end{aligned}$$

Theorem 3.2. *Let $n \geq 3$ be a positive integer. The first and second Zagreb eccentricity indices of the graph C_n^{2n-2} are*

$$E_1(C_n^{2n-2}) = \begin{cases} \frac{3}{4}n^3 + \frac{9}{2}n^2 + 5n - 8, & \text{if } n \text{ is even}\\ \frac{3}{4}n^3 + 3n^2 + \frac{7}{4}n - \frac{9}{2}, & \text{if } n \text{ is odd}\end{cases}$$

and

$$E_2(C_n^{2n-2}) = \begin{cases} \frac{3}{4}n^3 + \frac{7}{2}n^2 + 2n - 4, & \text{if } n \text{ is even}\\ \frac{3}{4}n^3 + 2n^2 - \frac{1}{4}n - \frac{3}{2}, & \text{if } n \text{ is odd.}\end{cases}$$

Proof. *Recall that the total number of vertices in C_n^{2n-2} is $3n-2$. Based on the number n of vertices corresponding to n carbon atoms of cycloalkenes, we consider the following two cases:*

Case (i) *n is even.*

In this case, the eccentricity of each vertex corresponding to a carbon atom is $\frac{n}{2}+1$. The eccentricity of each vertex corresponding to $2n-2$ hydrogen atoms is $\frac{n}{2}+2$. So we have

$$\begin{aligned}E_1(C_n^{2n-2}) =& \sum_{v_i \in V(C_n^{2n-2})} e_i^2\\ =&n\left(\frac{n}{2}+1\right)^2 + (2n-2)\left(\frac{n}{2}+2\right)^2\\ =&\frac{3}{4}n^3 + \frac{9}{2}n^2 + 5n - 8\end{aligned}$$

and

$$\begin{aligned}E_2(C_n^{2n-2}) =& \sum_{v_iv_j \in E(C_n^{2n-2})} e_ie_j\\ =&n\left(\frac{n}{2}+1\right)^2 + (2n-2)\left(\frac{n}{2}+1\right)\left(\frac{n}{2}+2\right)\\ =&\frac{3}{4}n^3 + \frac{7}{2}n^2 + 2n - 4.\end{aligned}$$

Case (ii) *n is odd.*

In this case, the eccentricity of each vertex corresponding to the carbon atom is $\frac{n-1}{2}+1$. *The eccentricity of each vertex corresponding to* $2n-2$ *hydrogen atoms is* $\frac{n-1}{2}+2$. *So we have*

$$\begin{aligned} E_1(C_n^{2n-2}) &= \sum_{v_i \in V(C_n^{2n-2})} e_i^2 \\ &= n\left(\frac{n-1}{2}+1\right)^2 + (2n-2)\left(\frac{n-1}{2}+2\right)^2 \\ &= \frac{3}{4}n^3 + 3n^2 + \frac{7}{4}n - \frac{9}{2} \end{aligned}$$

and

$$\begin{aligned} E_2(C_n^{2n-2}) &= \sum_{v_i v_j \in E(C_n^{2n-2})} e_i e_j \\ &= n\left(\frac{n-1}{2}+1\right)^2 + (2n-2)\left(\frac{n-1}{2}+1\right)\left(\frac{n-1}{2}+2\right) \\ &= \frac{3}{4}n^3 + 2n^2 - \frac{1}{4}n - \frac{3}{2}. \end{aligned}$$

Theorem 3.3. *Let* $n \geq 3$ *be a positive integer. Then the first and second Zagreb degree eccentricity indices of the graph* $G = C_n^{2n-2}$ *are*

$$DE_1(C_n^{2n-2}) = \begin{cases} \frac{3}{4}n^3 + \frac{21}{2}n^2 + 35n - 36, & \text{if } n \text{ is even} \\ \frac{1}{4}[3n^3 + 36n^2 + 103n - 114], & \text{if } n \text{ is odd.} \end{cases}$$

and

$$DE_2(C_n^{2n-2}) = \begin{cases} \frac{3}{4}n^3 + \frac{25}{2}n^2 + 44n - 55, & \text{if } n \text{ is even} \\ \frac{3}{4}n^3 + 11n^2 + \frac{131}{4}n - \frac{89}{2}, & \text{if } n \text{ is odd.} \end{cases}$$

Proof. *We know that* $|V(G)| = 3n-2$. *So we have the following cases.*

Case (i) *n is even.*

The eccentricity of each of the n vertices of G corresponding to a carbon atom of the cycloalkene is $\frac{n}{2}+1$. *Out of these n vertices, two have degree 3 each and* $n-2$ *have degree 4 each. The* $2n-2$ *pendant vertices of G correspond to the hydrogen atoms of the cycloalkene and have the same eccentricity* $\frac{n}{2}+2$. *Then*

$$\begin{aligned} DE_1(C_n^{2n-2}) &= \sum_{v_i \in V(C_n^{2n-2})} (e_i + d_i)^2 \\ &= (n-2)\left[\left(\frac{n}{2}+1\right)+4\right]^2 + 2\left[\left(\frac{n}{2}+1\right)+3\right]^2 + (2n-2)\left[\left(\frac{n}{2}+2\right)+1\right]^2 \\ &= \frac{3}{4}n^3 + \frac{21}{2}n^2 + 35n - 36 \end{aligned}$$

and

$$\begin{aligned}
DE_2(C_n^{2n-2}) = & \sum_{v_iv_j \in E(C_n^{2n-2})} (e_i+d_i)(e_j+d_j) \\
=&(n-3)\left[\left(\frac{n}{2}+1\right)+4\right]\left[\left(\frac{n}{2}+1\right)+4\right]+2\left[\left(\frac{n}{2}+1\right)+4\right]\left[\left(\frac{n}{2}+1\right)+3\right] \\
&+1\left[\left(\frac{n}{2}+1\right)+3\right]\left[\left(\frac{n}{2}+1\right)+3\right]+(2n-4)\left[\left(\frac{n}{2}+2\right)+1\right]\left[\left(\frac{n}{2}+1\right)+4\right] \\
&+2\left[\left(\frac{n}{2}+2\right)+1\right]\left[\left(\frac{n}{2}+1\right)+3\right] \\
=&\frac{3}{4}n^3+\frac{25}{2}n^2+44n-55.
\end{aligned}$$

Case (ii) *n is odd.*

The eccentricity of each of the n vertices of G corresponding to a carbon atom of the cycloalkene is $\frac{n-1}{2}+1$. Out of these n vertices, two have degree 3 each and $n-2$ have degree 4 each. The $2n-2$ pendant vertices of G correspond to the hydrogen atoms of cycloalkenes and have the same eccentricity $\frac{n-1}{2}+2$. Then

$$\begin{aligned}
DE_1(C_n^{2n-2}) = & \sum_{v_i \in V(C_n^{2n-2})} (e_i+d_i)^2 \\
=&(n-2)\left[\left(\frac{n-1}{2}+1\right)+4\right]^2+2\left[\left(\frac{n-1}{2}+1\right)+3\right]^2 \\
&+(2n-2)\left[\left(\frac{n-1}{2}+2\right)+1\right]^2 \\
=&\frac{1}{4}[3n^3+36n^2+103n-114]
\end{aligned}$$

and

$$\begin{aligned}
DE_2(C_n^{2n-2}) = & \sum_{v_iv_j \in E(C_n^{2n-2})} (e_i+d_i)(e_j+d_j) \\
=&(n-3)\left[\left(\frac{n-1}{2}+1\right)+4\right]\left[\left(\frac{n-1}{2}+1\right)+4\right] \\
&+2\left[\left(\frac{n-1}{2}+1\right)+4\right]\left[\left(\frac{n-1}{2}+1\right)+3\right] \\
&+1\left[\left(\frac{n-1}{2}+1\right)+3\right]\left[\left(\frac{n-1}{2}+1\right)+3\right] \\
&+(2n-4)\left[\left(\frac{n-1}{2}+2\right)+1\right]\left[\left(\frac{n-1}{2}+1\right)+4\right] \\
&+2\left[\left(\frac{n-1}{2}+2\right)+1\right]\left[\left(\frac{n-1}{2}+1\right)+3\right] \\
=&\frac{3}{4}n^3+11n^2+\frac{131}{4}n-\frac{89}{2}.
\end{aligned}$$

4 Topological indices of $C_n^{R_r}$

In this section, we construct general formulae for some topological indices of the chemical graph that is constructed by attaching an alkyl R_r instead of each hydrogen atom in the cycloalkenes.

We denote the group of alkyls by R_r, $r \in \mathbb{Z}^+$. For example R_1, R_2, R_3, $\ldots$ denote methyl, ethyl, propyl, $\ldots$, respectively, as shown in Fig. 4.1.

When we put an alkyl instead of each hydrogen atom in the cycloalkene, we get a new class of cycloalkenes. We denote the chemical graphs that are formed by attaching an R_r instead of each hydrogen atom in a cycloalkene by $C_n^{R_r}$ as shown in Fig. 4.2.

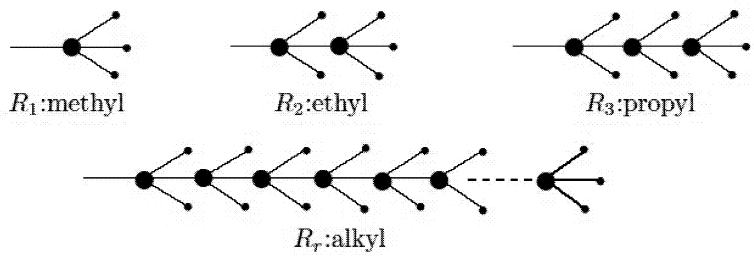

Figure 4.1 The first few alkyls

Fig. 4.2 represents the molecular structure of $C_n^{R_r}$ and Fig. 4.3 represents the corresponding molecular graph of $C_n^{R_r}$. The total number of vertices in the molecular structure and molecular graph are naturally equal. We calculate some degree based and eccentricity based topological indices of the graph shown in Fig. 4.3 in what follows.

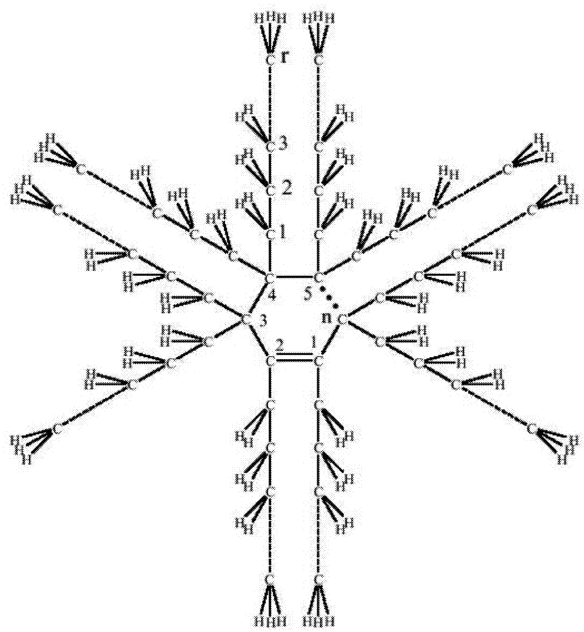

Figure 4.2 Molecular structure of $C_n^{R_r}$

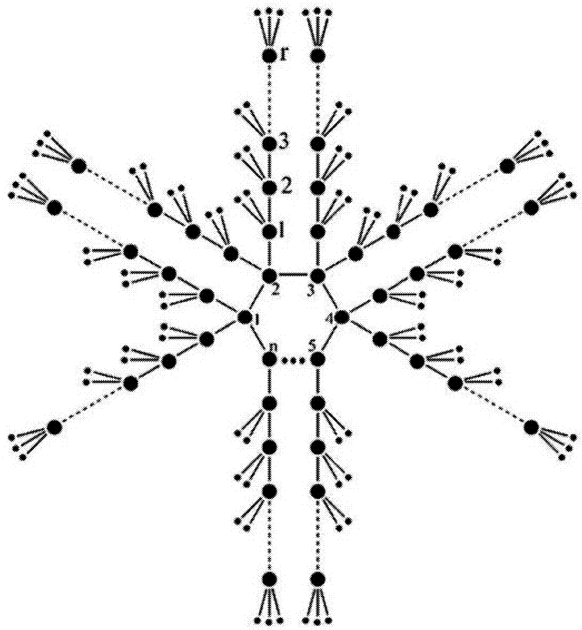

Figure 4.3 Molecular graph representing $C_n^{R_r}$

Theorem 4.1. *Let n and r be positive integers with $n \geq 3$. Then the first and second Zagreb indices of a graph $C_n^{R_r}$ are $(36r+18)n-(36r+16)$ and $(48r+24)n-(48r+31)$.*

Proof. *In graph $G = C_n^{R_r}$, $|V(G)| = 6nr + 3n - 6r - 2$. It has $n + 2nr - 2r$ vertices corresponding to the carbon atoms of $C_n^{R_r}$, n of them represent vertices of the cycle, out of which two have degree 3 and the remaining $n - 2$ have degree 4. The other $2nr - 2r$ vertices not on the cycle have the same degree 4. G also has $4nr + 2n - 4r - 2$ pendant vertices corresponding to the hydrogen atoms of $C_n^{R_r}$. Then*

$$
\begin{aligned}
M_1(C_n^{R_r}) = & \sum_{v_i \in V(C_n^{R_r})} d_i^2 \\
=& (n + 2nr - 2r - 2)(4^2) + 2(3^2) + (4nr + 2n - 4r - 2)(1^2) \\
=& (36r + 18)n - (36r + 16)
\end{aligned}
$$

and

$$
\begin{aligned}
M_2(C_n^{R_r}) = & \sum_{v_i v_j \in E(C_n^{R_r})} d_i d_j \\
=& (n-3)(4)(4) + 2(4)(3) + 1(3)(3) + (2n-4)(4)(4) + 2(3)(4) \\
& + (2n-2)(r-1)(4)(4) + (2r+1)(2n-2)(1)(4) \\
=& (48r + 24)n - (48r + 31).
\end{aligned}
$$

Theorem 4.2. *Let n and r be positive integers with $n \geq 3$. Then the first Zagreb* *eccentricity index of the graph* $G = C_n^{R_r}$ *is*

$$E_1(C_n^{R_r}) = \begin{cases} \frac{3}{2}n^3\left(r+\frac{1}{2}\right)+3n^2\left(3r^2+\frac{11}{2}r+\frac{3}{2}\right)+n\left(14r^3+39r^2+30r+5\right) \\ -\left(14r^3+47r^2+45r+8\right), & \text{if } n \text{ is even} \\ \frac{3}{2}n^3\left(r+\frac{1}{2}\right)+3n^2\left(3r^2+\frac{9}{2}r+1\right)+n\left(14r^3+30r^2+\frac{33}{2}r+\frac{7}{4}\right) \\ -\left(14r^3+38r^2+\frac{59}{2}r+\frac{9}{2}\right), & \text{if } n \text{ is odd.} \end{cases}$$

Proof. *Consider the graph* $G = C_n^{R_r}$. *Then* $|V(G)| = 6nr + 3n - 6r - 2$. *Here* $n + 2nr - 2r$ *vertices of* G *correspond to the carbon atoms of* $C_n^{R_r}$. *In Table 1, the eccentricities of the vertices of* $C_n^{R_r}$ *are shown. We consider the following cases.*

vertex corresponding to	number of vertices	eccentricity	
		for even n	for odd n
C on a cycle	n	$\frac{n}{2}+r+1$	$\frac{n-1}{2}+r+1$
C not on cycle	$2nr-2r$	$\frac{n}{2}+r+1+i$, $1 \le i \le r$	$\frac{n-1}{2}+r+1+i$, $1 \le i \le r$
H	$4nr+2n-4r-2$	$\frac{n}{2}+r+i+2$, $1 \le i \le r$	$\frac{n-1}{2}r+i+2$, $1 \le i \le r$

Table 1: Eccentricities of the vertices of $C_n^{R_r}$

Case (i) *n is even.*

$$\begin{aligned} E_1(C_n^{R_r}) &= \sum_{v_i \in V(C_n^{R_r})} e_i^2 \\ &= n\left(\frac{n}{2}+r+1\right)^2 + (2n-2)\sum_{i=1}^{r}\left(\frac{n}{2}+r+1+i\right)^2 \\ &\quad + (2n-2)2\sum_{i=1}^{r}\left(\frac{n}{2}+r+i+2\right)^2 + (2n-2)\left(\frac{n}{2}+r+r+2\right)^2 \\ &= \frac{3}{2}n^3\left(r+\frac{1}{2}\right)+3n^2\left(3r^2+\frac{11}{2}r+\frac{3}{2}\right) \\ &\quad + n\left(14r^3+39r^2+30r+5\right)-\left(14r^3+47r^2+45r+8\right). \end{aligned}$$

Case (ii) *n is odd.*

$$
\begin{aligned}
E_1(C_n^{R_r}) &= \sum_{v_i \in V(C_n^{R_r})} e_i^2 \\
&= n\left(\frac{n-1}{2}+r+1\right)^2 + (2n-2)\sum_{i=1}^{r}\left(\frac{n-1}{2}+r+1+i\right)^2 \\
&\quad + (2n-2)2\sum_{i=1}^{r}\left(\frac{n-1}{2}+r+i+2\right)^2 + (2n-2)\left(\frac{n-1}{2}+r+r+2\right)^2 \\
&= \frac{3}{2}n^3\left(r+\frac{1}{2}\right) + 3n^2\left(3r^2+\frac{9}{2}r+1\right) + n\left(14r^3+30r^2+\frac{33}{2}r+\frac{7}{4}\right) \\
&\quad - \left(14r^3+38r^2+\frac{59}{2}r+\frac{9}{2}\right).
\end{aligned}
$$

Theorem 4.3. *Let n and r be positive integers with $n \geq 3$. The second Zagreb eccentricity index of a graph $G = C_n^{R_r}$ is*

$$
E_2(C_n^{R_r}) = \begin{cases}
\frac{3}{2}n^3\left(r+\frac{1}{2}\right) + n^2\left(9r^2+\frac{27}{2}r+\frac{7}{2}\right) + 2n\left(7r^3+15r^2+8r+1\right) \\
-\left(14r^3+38r^2+28r+4\right), & \text{if } n \text{ is even} \\
\frac{3}{2}n^3\left(r+\frac{1}{2}\right) + n^2\left(9r^2+\frac{21}{2}r+2\right) + n\left(14r^3+21r^2+\frac{11}{2}r-\frac{1}{4}\right) \\
-\left(14r^3+\frac{28}{3}r^2+\frac{31}{2}r+\frac{3}{2}\right), & \text{if } n \text{ is odd.}
\end{cases}
$$

Proof. *In view of the proof of Theorem 4.2 and Table 1, we consider the following cases.*

Case (i) *n is even.*

$$
\begin{aligned}
E_2(C_n^{R_r}) &= \sum_{v_i v_j \in E(C_n^{R_r})} e_i e_j \\
&= n\left(\frac{n}{2}+r+1\right)\left(\frac{n}{2}+r+1\right) + (2n-2)\left(\frac{n}{2}+r+1\right)\left(\frac{n}{2}+r+2\right) \\
&\quad + (2n-2)\sum_{i=1}^{r-1}\left(\frac{n}{2}+r+1+i\right)\left(\frac{n}{2}+r+i+2\right) \\
&\quad + (2n-2)2\sum_{i=1}^{r}\left(\frac{n}{2}+r+i+2\right)\left(\frac{n}{2}+r+1+i\right) \\
&\quad + (2n-2)\left(\frac{n}{2}+r+r+2\right)\left(\frac{n}{2}+r+1+r\right) \\
&= \frac{3}{2}n^3\left(r+\frac{1}{2}\right) + n^2\left(9r^2+\frac{27}{2}r+\frac{7}{2}\right) + 2n\left(7r^3+15r^2+8r+1\right) \\
&\quad - \left(14r^3+38r^2+28r+4\right).
\end{aligned}
$$

Case (ii) *n is odd.*

$$
\begin{aligned}
E_2(C_n^{R_r}) = &\sum_{v_iv_j \in E(C_n^{R_r})} e_i e_j \\
=&n\left(\frac{n-1}{2}+r+1\right)\left(\frac{n-1}{2}+r+1\right) \\
&+(2n-2)\left(\frac{n-1}{2}+r+1\right)\left(\frac{n-1}{2}+r+2\right) \\
&+(2n-2)\sum_{i=1}^{r-1}\left(\frac{n-1}{2}+r+1+i\right)\left(\frac{n-1}{2}+r+i+2\right) \\
&+(2n-2)2\sum_{i=1}^{r}\left(\frac{n-1}{2}+r+i+2\right)\left(\frac{n-1}{2}+r+1+i\right) \\
&+(2n-2)\left(\frac{n-1}{2}+r+r+2\right)\left(\frac{n-1}{2}+r+1+r\right) \\
=&\frac{3}{2}n^3\left(r+\frac{1}{2}\right)+n^2\left(9r^2+\frac{21}{2}r+2\right)+n\left(14r^3+21r^2+\frac{11}{2}r-\frac{1}{4}\right) \\
&-\left(14r^3+\frac{28}{3}r^2+\frac{31}{2}r+\frac{3}{2}\right).
\end{aligned}
$$

Theorem 4.4. *Let n and r be positive integers with $n \geq 3$. Then the first Zagreb degree eccentricity index of the graph $G = C_n^{R_r}$ is*

$$
DE_1(C_n^{R_r}) = \begin{cases}
\frac{3}{2}n^3\left(r+\frac{1}{2}\right)+n^2\left(9r^2+\frac{57}{2}r+\frac{21}{2}\right)+n\left(14r^3+75r^2+114r+35\right) \\
-\left(14r^3+83r^2+137r+36\right), & \text{if } n \text{ is even} \\
\frac{3}{2}n^3\left(r+\frac{1}{2}\right)+n^2\left(9r^2+\frac{51}{2}r+9\right)+n\left(14r^3+66r^2+\frac{177}{2}r-\frac{103}{4}\right) \\
-\left(14r^3+74r^2+\frac{219}{2}r+\frac{57}{2}\right), & \text{if } n \text{ is odd.}
\end{cases}
$$

Proof. *In graph $G = C_n^{R_r}$, $|V(G)| = 6nr + 3n - 6r - 2$. We consider the following cases.*

Case (i) *n is even.*

$n + 2nr - 2r$ vertices of G correspond to the carbon atoms of $C_n^{R_r}$, n of them represent vertices of the cycle that have the same eccentricity $\frac{n}{2}+r+1$ such that two of them have degree 3 and the remaining $n-2$ have degree 4. The remaining $2nr-2r$ vertices not on the cycle have the same degree 4 and have the eccentricity $\frac{n}{2}+r+1+i$, $i = 1, 2, 3, \ldots, r$, respectively. It also contains $4nr + 2n - 4r - 2$ pendant vertices corresponding to the hydrogen atoms of $C_n^{R_r}$ having the eccentricity $\frac{n}{2}+r+i+2$, $i = 1, 2, 3, \ldots, r$, respectively. Then,

$$\begin{aligned}
DE_1(C_n^{R_r}) = &\sum_{v_i \in V(C_n^{R_r})} (e_i + d_i)^2 \\
=&(n-2)\left[\left(\frac{n}{2}+r+1\right)+4\right]^2 + 2\left[\left(\frac{n}{2}+r+1\right)+3\right]^2 \\
&+ (2n-2)\sum_{i=1}^{r}\left[\left(\frac{n}{2}+r+1+i\right)+4\right]^2 \\
&+ (2n-2)2\sum_{i=1}^{r}\left[\left(\frac{n}{2}+r+i+2\right)+1\right]^2 \\
&+ (2n-2)\left[\left(\frac{n}{2}+r+r+2\right)+1\right]^2 \\
=&\frac{3}{2}n^3\left(r+\frac{1}{2}\right)+n^2\left(9r^2+\frac{57}{2}r+\frac{21}{2}\right)+n\left(14r^3+75r^2+114r+35\right) \\
&-\left(14r^3+83r^2+137r+36\right).
\end{aligned}$$

Case (ii) *n is odd.*

$n+2nr-2r$ vertices of G correspond to the carbon atoms of $C_n^{R_r}$, n of them represent vertices of the cycle that have the same eccentricity $\frac{n-1}{2}+r+1$ such that two of them have degree 3 and the remaining $n-2$ have degree 4. The remaining $2nr-2r$ vertices not on the cycle have the same degree 4 and have eccentricity $\frac{n-1}{2}+r+1+i$, $i=1,2,3,\ldots,r$, respectively. It also contains $4nr+2n-4r-2$ pendant vertices corresponding to the hydrogen atoms of $C_n^{R_r}$, having the eccentricity $\frac{n-1}{2}+r+i+2$, $i=1,2,3,\ldots,r$, respectively. Then,

$$\begin{aligned}
DE_1(C_n^{R^r}) = &\sum_{v_i \in V(C_n^{R^r})} (e_i + d_i)^2 \\
=&(n-2)\left[\left(\frac{n-1}{2}+r+1\right)+4\right]^2 + 2\left[\left(\frac{n-1}{2}+r+1\right)+3\right]^2 \\
&+ (2n-2)\sum_{i=1}^{r}\left[\left(\frac{n-1}{2}+r+1+i\right)+4\right]^2 \\
&+ (2n-2)2\sum_{i=1}^{r}\left[\left(\frac{n-1}{2}+r+i+2\right)+1\right]^2 \\
&+ (2n-2)\left[\left(\frac{n-1}{2}+r+r+2\right)+1\right]^2 \\
=&\frac{3}{2}n^3\left(r+\frac{1}{2}\right)+n^2\left(9r^2+\frac{51}{2}r+9\right)+n\left(14r^3+66r^2+\frac{177}{2}r-\frac{103}{4}\right) \\
&-\left(14r^3+74r^2+\frac{219}{2}r+\frac{57}{2}\right).
\end{aligned}$$

Theorem 4.5. *Let n and r be positive integers with $n \geq 3$. The second Zagreb* *degree eccentricity index of the graph* $G = C_n^{R_r}$ *is*

$$DE_2(C_n^{R_r}) = \begin{cases} \frac{3}{2}n^3\left(r+\frac{1}{2}\right)+n^2\left(9r^2+\frac{63}{2}r+\frac{25}{2}\right)+n\left(14r^3+84r^2+136r+44\right) \\ -\left(14r^3+85r^2+84r-163\right), & \text{if } n \text{ is even} \\ \frac{3}{2}n^3\left(r+\frac{1}{2}\right)+n^2\left(9r^2+\frac{57}{2}r+11\right)+n\left(14r^3+75r^2+\frac{215}{2}r+\frac{131}{4}\right) \\ -\left(14r^3+83r^2+\frac{267}{2}r+\frac{101}{2}\right), & \text{if } n \text{ is odd.} \end{cases}$$

Proof. *In the graph* G, $|V(G)| = 6nr+3n-6r-2$. *We consider the following cases.*

Case (i) n *is even.*

From Case (i) of the proof of Theorem 4.4, we have

$$\begin{aligned} DE_2(C_n^{R_r}) = & \sum_{v_iv_j \in E(C_n^{R_r})} (e_i+d_i)(e_j+d_j) \\ =&(n-3)\left[\left(\frac{n}{2}+r+1\right)+4\right]\left[\left(\frac{n}{2}+r+1\right)+4\right] \\ &+2\left[\left(\frac{n}{2}+r+1\right)+4\right]\left[\left(\frac{n}{2}+r+1\right)+3\right] \\ &+\left[\left(\frac{n}{2}+r+1\right)+3\right]\left[\left(\frac{n}{2}+r+1\right)+3\right] \\ &+(2n-4)\left[\left(\frac{n}{2}+r+1\right)+4\right]\left[\left(\frac{n}{2}+r+2\right)+4\right] \\ &+2\left[\left(\frac{n}{2}+r+1\right)+3\right]\left[\left(\frac{n}{2}+r+2\right)+4\right] \\ &+(2n-2)\sum_{i=1}^{r-1}\left[\left(\frac{n}{2}+r+1+i\right)+4\right]\left[\left(\frac{n}{2}+r+i+2\right)+4\right] \\ &+(2n-2)2\sum_{i=1}^{r}\left[\left(\frac{n}{2}+r+i+2\right)+1\right]\left[\left(\frac{n}{2}+r+1+i\right)+4\right] \\ &+(2n-2)\left[\left(\frac{n}{2}+r+r+2\right)+1\right]\left[\left(\frac{n}{2}+r+1+r\right)+4\right] \\ =&\frac{3}{2}n^3\left(r+\frac{1}{2}\right)+n^2\left(9r^2+\frac{63}{2}r+\frac{25}{2}\right)+n\left(14r^3+84r^2+136r+44\right) \\ &-\left(14r^3+85r^2+84r-163\right). \end{aligned}$$

Case (ii) n *is odd.*

From Case (ii) of the proof of Theorem 4.4, we have

$$
\begin{aligned}
DE_2(C_n^{R_r}) = & \sum_{v_iv_j \in E(C_n^{R_r})} (e_i + d_i)(e_j + d_j) \\
=&(n-3)\left[\left(\frac{n-1}{2}+r+1\right)+4\right]\left[\left(\frac{n-1}{2}+r+1\right)+4\right] \\
&+2\left[\left(\frac{n-1}{2}+r+1\right)+4\right]\left[\left(\frac{n-1}{2}+r+1\right)+3\right] \\
&+\left[\left(\frac{n-1}{2}+r+1\right)+3\right]\left[\left(\frac{n-1}{2}+r+1\right)+3\right] \\
&+(2n-4)\left[\left(\frac{n-1}{2}+r+1\right)+4\right]\left[\left(\frac{n-1}{2}+r+2\right)+4\right] \\
&+2\left[\left(\frac{n-1}{2}+r+1\right)+3\right]\left[\left(\frac{n-1}{2}+r+2\right)+4\right] \\
&+(2n-2)\sum_{i=1}^{r-1}\left[\left(\frac{n-1}{2}+r+1+i\right)+4\right]\left[\left(\frac{n-1}{2}+r+i+2\right)+4\right] \\
&+(2n-2)2\sum_{i=1}^{r}\left[\left(\frac{n-1}{2}+r+i+2\right)+1\right]\left[\left(\frac{n-1}{2}+r+1+i\right)+4\right] \\
&+(2n-2)\left[\left(\frac{n-1}{2}+r+r+2\right)+1\right]\left[\left(\frac{n-1}{2}+r+1+r\right)+4\right] \\
=&\frac{3}{2}n^3\left(r+\frac{1}{2}\right)+n^2\left(9r^2+\frac{57}{2}r+11\right)+n\left(14r^3+75r^2+\frac{215}{2}r+\frac{131}{4}\right) \\
&-\left(14r^3+83r^2+\frac{267}{2}r+\frac{101}{2}\right).
\end{aligned}
$$

Conclusion

In this paper, we computed the first and second Zagreb indices, first and second Zagreb eccentricity indices and first and second Zagreb degree eccentricity indices of molecular graphs of cycloalkenes and $C_n^{R_r}$ with the help of graph theory and mathematical derivation. It is interesting to investigate this index for other chemical structures via their molecular graphs.

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