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Eccentric Connectivity Index of Chemical Trees

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Abstract. Let $G = (V, E)$ be a simple connected molecular graph. In such a simple molecular graph, vertices and edges are depicted atoms and chemical bonds respectively, we refer to the sets of vertices by $V\,(G)$ and edges by$E\,(G)$.If $d(u, v)$ be distance between two vertices $u, v \in V(G)$ and can be defined as the length of a shortest path joining them. Then, the eccentricity connectivity index (ECI) of a molecular graph G is$\xi(G) = \sum_{v \in V(G)} d(v)\, ec(v)$, where $d(v)$ is degree of a vertex $v \in V(G)$. $ec(v)$ is the length of a greatest path linking to another vertex of v. In this study, we focus the general formula for the eccentricity connectivity index (ECI) of some chemical trees as alkenes.

INTRODUCTION

In chemistry, a molecular structure embodies the topology of a molecule, by concerning how the atoms are joined. This could be modeled by a graph, where the points and edges represent atoms and bonds, respectively. The variables are derived from this graph theoretic sample of chemical forms that being employed not only in studies of QSAR concerning molecular structure and pharmaceutical drug one, but also in the atmosphere hazard chemicals assessment.

A large number of topological indices had been investigated and used. Firstly, and the most famous, the Wiener index, was founded in the late 1940s in end devour to analyze the chemical properties of alkanes group [1]. It is a distance based index, whose chemical applications and mathematical properties have been extensively studied. Many other indices are known, and nowadays, indices like the eccentric distance sum and the adjacency cum eccentricity-based eccentric connectivity index have been investigated [2, 3, 4, 5, 6, 7, 8, 9 and 10]. These topological indices had been stated to provide a high degree of possibility of pharmaceutical properties, and might lead for the improvement of potent and safe anti-HIV compound. Revision these indices have also been concerned. For instance, the augmented eccentric connectivity index [11, 12 and 13] and the super augmented eccentric connectivity index [14] have been investigated to be beneficial indicators in chemistry study.

In this study, we find the general formula for the eccentricity connectivity index $\xi(G)$ of a new class of chemical trees.

ECCENTRIC CONNECTIVITY INDEX OF SOME CLASSES OF CHEMICAL TREES

In this section, we establish the general formula for the eccentric connectivity index (ECI) of some classes of chemical trees.

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Alkenes are hydrocarbons with at least one double bond between the carbon atoms. They will be called as terminal alkenes if the double bond if present in the end of the carbon chain. They have the general formula of C_nH_{2n}.

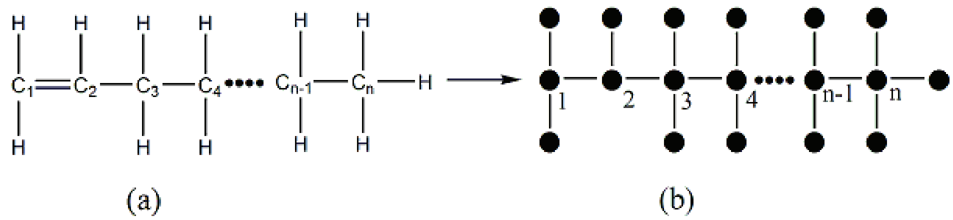


FIGURE 1. (a) is molecular structure of classes of chemical trees (Alkenes C_nH_{2n}); (b) is molecular graph representing the chemical trees (Alkenes).

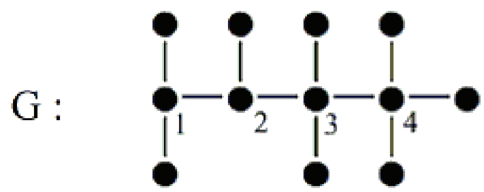
Theorem 2.1. Let *n* be the integer number. Then the eccentric connectivity index of the graph G associated with C_nH_{2n} (Alkenes) (see Fig.1. b), is

$$\xi(G) = \begin{cases} \frac{1}{2}(9n^2 + 6n + 4)\,; & for\ n\ is\ even, n \geq 4 \\ \frac{1}{2}(9n^2 + 6n + 1)\,; & for\ n\ is\ odd, n \geq 3 \end{cases}$$

Proof: We will prove this theorem by mathematical induction, we have two cases:

Case.1. If n is even:

Let $n = 4$ then G is associated with C_4H_8. The graph is as follows:



Thus $\xi(C_4H_8) = (5)(1)(5) + (10)(4) + (7)(3) = 86$.

Hence it is true that

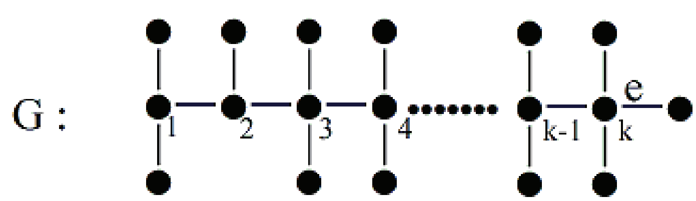
$$\xi(G) = \tfrac{1}{2}(9n^2 + 6n + 4);\ n{=}4.$$

Suppose that the hypothesis is true when $n = k$, $(k \geq 4)$, k is even. That is the eccentric connectivity index for the graph G associated in C_kH_{2k} is given by:

$$\xi(G) = \tfrac{1}{2}(9k^2 + 6k + 4).$$

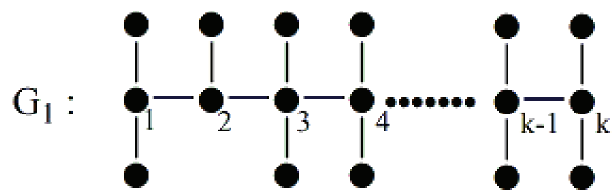
Construct the graph G associated with $C_{k+2}H_{2k+4}$ as follows:

The graph G related with C_kH_{2k}has the form:



where C_i refers the stance of the carbon vertex at the i^{th} the position, and e the edge joining the vertex k of graph G with the vertex corresponding to the end hydrogen vertex H.

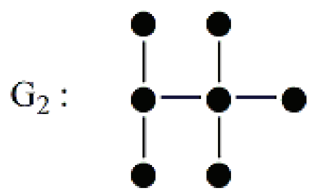
Let G_1 be the graph got from G by sweep the edge e that is:



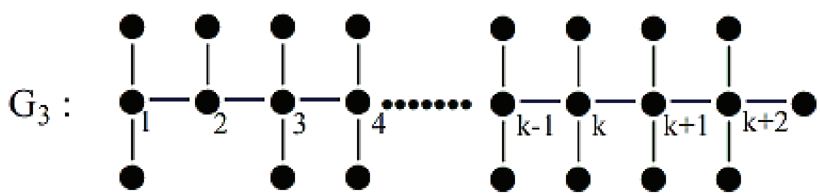
For the graph G_1,

$$\xi(G_1) = \xi(G) - (k+1) = \frac{1}{2}(9k^2 + 6k + 4) - (k+1) = \frac{9}{2}k^2 + 2k + 1.$$

Let G_2 be the graph



We construct the graph G_1 by connecting the k^{th} vertex in $G_1$with the vertex in G_2. We obtain the graph G_3 as follows



The $k+2^{th}$ vertex is adjacent to five other vertices in G_3. Now, $G_3$is the graph associated with the molecular structure of $C_{k+2}H_{2k+4}$.

In this case, we will get an increase in the eccentricity to $(\frac{1}{2}k+1)$ of carbon vertices, where $\left(\frac{1}{2}k\right)$ increases by 2 [$(\frac{1}{2}k-2)$ of them have degree 4 and just two have degree 3], and one vertex increase by 1. Also we will get an increase in eccentricity to k+1 of vertices hydrogen, where k-1 of them have increase by 2 and just two vertices increase by 1.

Thus

$$\xi(G_{k+2}H_{2k+6}) = \xi(G_1) + \xi(G_2) + \xi(increases)$$

$$= \left(\frac{9}{2}k^2 + 2k + 1\right) + (13k + 25) + \left(\frac{1}{2}k - 2\right)(4)(2) + (2)(3)(2) + (1)(4)(1)$$

$$+(k-1)(1)(2) + (2)(1)(1)$$

$$= \frac{9}{2}k^2 + 21k + 26.$$

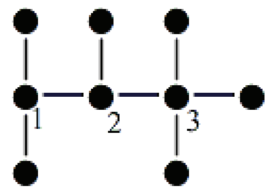
Therefore the assertion is true when $n = k + 2$.

Since the assertion is true when $n = 4$, also with the assumption that it is true for $n = k$, and it is shown that it is true for $n = k + 2$, it follows that

$\xi(G) = \frac{1}{2}(9n^2 + 6n + 4)$, if G is the graph (b) in Fig. 1, for all $n \geq 4$, n is even.

Case.2. If n is odd:

Let $n = 3$ then $G = C_3H_6$, whose graph as follows:



Thus $\xi(G) = (5)(1)(4) + (8)(3) + (3)(2) = 50$.

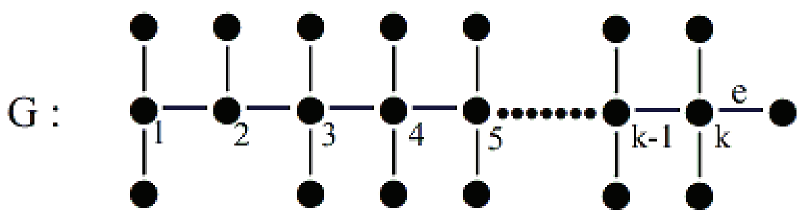
Hence it is true that $\xi(G) = \frac{1}{2}(9n^2 + 6n + 1)$, when $n = 3$.

Suppose that the hypothesis is true when $n = k$, ($k \geq 3$), k is odd. That is the eccentric connectivity index for the graph G related in C_kH_{2k} is given by:

$$\xi(G) = \frac{1}{2}(9k^2 + 6k + 1).$$

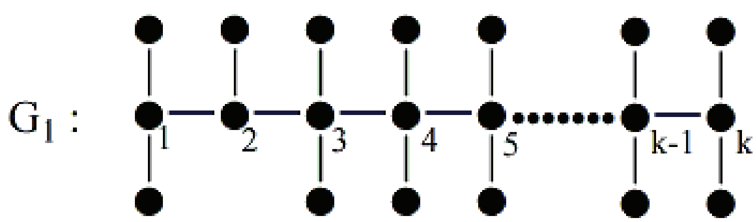
Construct the graph G related with $C_{k+2}H_{2k+4}$ as follows:

The graph G related with C_kH_{2k} has the form:



Where C_i refers the position of the carbon vertex at the i^{th} the position, and e the edge connecting the vertex k of graph G with the vertex corresponding to the end hydrogen vertex H.

Let G_1 be the graph obtained from G by removing the edge e that is:

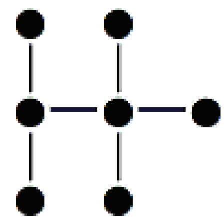


For the graph G_1,

$$\xi(G_1) = \xi(G) - (k + 1) = \frac{1}{2}(9k^2 + 6k + 1) - (k + 1) = \frac{9}{2}k^2 + 2k - \frac{1}{2}.$$

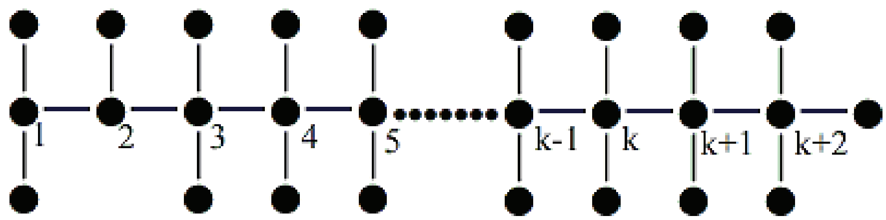
Let G_2 be the graph

G_2 :



We construct the graph G_3 by connecting the k^{th} vertex in $G_1$with the vertex in G_2. We obtain the graph G_3 as follows

G_3 :



The $k+2^{th}$ vertex is adjacent to five other vertices in G_3. Now, $G_3$is the graph associated with the molecular structure of $C_{k+2}H_{2k+4}$.

In this case, we will get an increase in the eccentricity to $\frac{1}{2}(k+1)$ of vertices carbon, increase by 2 [$\frac{1}{2}(k-3)$ of them have degree 4 and just two have degree 3]. Also we will get an increase in eccentricity by 2 to k of vertices hydrogen.

Thus

$$\xi(G_{k+2}H_{2k+6}) = \xi(G_1) + \xi(G_2) + \xi(increases)$$

$$= \left(\frac{9}{2}k^2 + 2k - \frac{1}{2}\right) + (13k + 25) + \frac{1}{2}(k-3)(4)(2) + (2)(3)(2) + (k)(1)(2)$$

$$= \frac{9}{2}k^2 + 21k + \frac{49}{2}.$$

Therefore the assertion is true for $n = k + 2$.

Since the assertion is true for $n = 3$, also with the assumption that it is true for $n = k$, and it is shown that it is true for $n = k + 2$, it follows that

$\xi(G) = \frac{1}{2}(9n^2 + 6n + 1)$, if G is the graph (b) in Fig. 1, for $n \geq 3$, n is odd. □

CONCLUSION

In this paper, we computed the eccentric connectivity index of molecular graphs of chemical trees. It is interesting to investigate this index for other chemical structures via their molecular graphs. The characterization of graphs with extremism eccentric connectivity index has been an active area of research and we hope to consider this problem in future. We close this paper with following question: Which graphs will attain the maximum or minimum eccentric connectivity index?

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