# On leap eccentric connectivity index of some chemical trees

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**ABSTRACT**

The 2-degree of a vertex v of a simple graph G is the number of vertices which are at distance two from v in G and is denoted by d2(v). In this article, we compute exact values of a recent eccentricity-based topological index called Leap eccentric connectivity index (LECI), which is defined as the sum of product of 2-degree and eccentricity of every vertex in G, for some special classes of chemical trees. Also we discuss some of its applications in chemical structures such as alkanes.

**KEYWORDS:** Topological indices, Leap eccentricity connectivity index, Alkanes, Chemical trees

## 1 INTRODUCTION

A topological index, in general, is a function TI from collection of all graphs G onto the set of positive real numbers R, which characterizes the topology of a molecular graph $G$ of a chemical structure. Also several topological indices have been extensively applied in QSAR and QSPR studies in Inorganic Chemistry. Zagreb indices and Wiener index are considered as oldest topological indices and even now they have some influence with the new topological invariants. It is possible do a detailed survey on such indices [3]. In general, topological indices are widely classified into two types: Degree-based and distance-based indices. There are abundant research articles in literature related to both of these categories. Of all those indices, eccentricity-based topological indices have been a prime focus of researchers in Mathematical Chemistry. Recently, A.M. Naji et al. [6,9] have introduced one such eccentricity-based topological index, called LECI followed by their seminal paper on Leap Zagreb indices [8].

Raad et al. [4] studied eccentric connectivity index of unicylic type graphs with some applications in cycloalkanes. Also Raad [5] accompanied by a team of researchers studied a new topological invariant known as Multiplicative leap Zagreb indices and obtained exact values for some special classes of thorny graphs. To study thorny graphs with other topological indices, one may refer to further sources [8, 11, 12-16]. As a follow-up study, we have addressed the recent 2-degree and eccentricity-based topological index, namely, LECI on chemical trees. Also we have discussed some applications of these results related to chemical compounds as group of alkanes. Before we proceed to discuss the main results, we represent the following preliminary definitions and results.

**Definition 1** ([9, 2]): The 2-degree of a vertex v in a graph G is defined as $d_2(v) = \{u \in V(G) : d(u,v) = 2\}$. Some authors refer to this one as Zagreb connection number and denote it as $\tau(v)$. However, we follow the notation 2-degree in line with previous research [9].

The following definition is about three types of distance-based indices, collectively known as Leap Zagreb indices.

**Definition 2** ([9]): The first leap Zagreb index of a graph G is denoted by $LM_1(G)$ and defined as $LM_1(G) = \sum_{v \in V(G)} [d_2(v)]^2$.

The second leap Zagreb index of G is denoted by $LM_2(G)$ and defined as $LM_2(G) = \sum_{uv \in E(G)} d_2(u) d_2(v)$.

The third leap Zagreb index of G is defined as $LM_3(G) = \sum_{v \in V(G)} \deg(v) d_2(v)$. In litearure, this index is also known as Zagreb connection index of a graph G.

**Definition 3**: Let G be a simple connected graph on $n$ vertices $\{v_1, v_2, ..., v_n\}$. Let $\{p_1, p_2, ..., p_n\}$ be a sequence of positive integers. Then a thorny graph $G^* = G^*(p_1, p_2, ..., p_n)$ is a graph obtained from G by attaching $p_i$ pendant vertices (known as thorns) to every vertex $v_i$ of G, $1 \le i \le n$.

## 2 RESULTS AND DISCUSSION

A.M.Naji et al. [10] defined the following novel invariant called LECI of a graph. Also they studied this new topological index on graphs resulting from some graph operations.

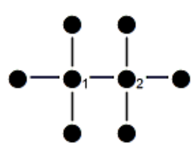
**Theorem 1** Let $n$ be a positive integer. Then the leap eccentric connectivity index of the graph G associated with $C_nH_{2n+2}$ is

$$L\xi(G) = \begin{cases} 9n^2 + 12n + 6\,; & if\ n\ is\ even, n \ge 2 \\ 9n^2 + 12n + 3\,; & if\ n\ is\ odd, n \ge 1 \end{cases}$$

**Proof:** We prove by the induction on n, where n is the number carbon atoms.

**Case 1:** If n is even

Let $n = 2$ then G is associated with $C_2H_6$. The graph is as follows:




Thus

$L\xi(C_2H_6) = (6)(3)(3) + (2)(3)(2) = 66$

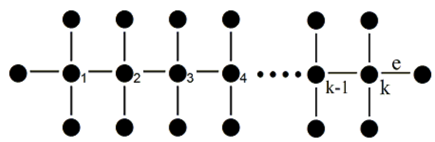
Hence it is true that

$L\xi(G) = 9n^2 + 12n + 6$, when $n = 2$

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

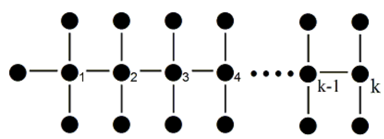
$$L\xi(G) = 9k^2 + 12k + 6$$

Construct the graph G associated with $C_{k+2}H_{2k+6}$ as follows:
The graph G related with $C_kH_{2k+2}$ has the form:




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

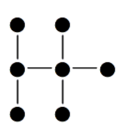
Let $G_1$ be the graph obtained from G by removing the edge e that is



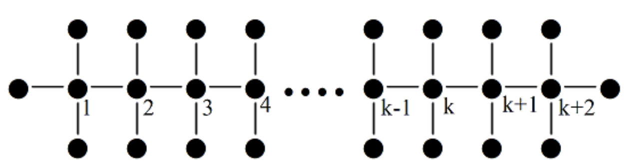

For the graph $G_1$ we get

$$L\xi(G_1) = L\xi(G_k) - 3(k+1) = 9k^2 + 9k + 3$$

Let $G_2$ be the graph



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:



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 $C_{k+2}H_{2k+6}$.

In this case, we will get an increase in the eccentricity to $\frac{1}{2}k+1$ of carbon vertices, where $\frac{1}{2}k$ increase by 2, and one vertex increase by 1. Also we will get an increase in eccentricity to $k+1$ of hydrogen vertices by two, and just two vertices increase by 1
Thus

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

$$= (9k^2+9k+3) + (27k+51) + \left(\frac{1}{2}k-1\right)(6)(2) + (1)(6)(1)$$

$$+(k+1)(3)(2) + (3)(2)$$

$$= 9k^2 + 48k + 66$$

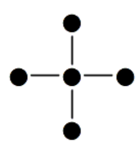
Therefore the assertion is true when $n = k+2$.

Since the assertion is true when $n = 2$, 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

$$L\xi(G) = 9n^2 + 12n + 6, \text{ for all n even, } n \geq 2.$$

**Case 2:** If n is odd

Let $n = 1$ then G is associated with $C_1H_4$. The graph is as follows:



Thus

$$L\xi(C_1H_4) = (4)(3)(2) = 24$$

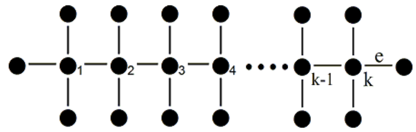
Hence it is true that

$$L\xi(G) = 9n^2 + 12n + 3, \text{ when } n = 1$$

Suppose that the hypothesis is true when $n = k$, $k \geq 1$, k is odd. That is the eccentric connectivity index for the graph G associated with $C_kH_{2k+2}$ is given by:

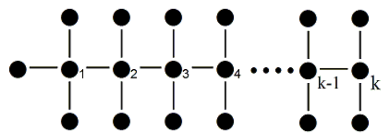
$$\xi(G) = 9k^2 + 12k + 3$$

Construct the graph G associated with $C_{k+2}H_{2k+6}$ as follows:
The graph G related with $C_kH_{2k+2}$ has the form:




where $C_i$ denotes the position of the carbon vertex at the $i^{th}$ position, and e the edge connecting the vertex k in graph G with the vertex corresponding to the end hydrogen vertex H

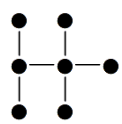
Let $G_1$ be the graph obtained from G by removing the edge e that is:



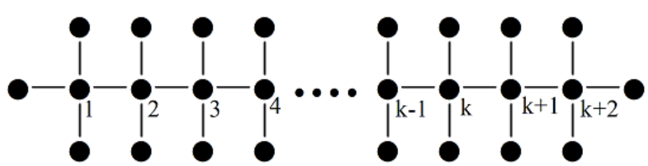

For the graph $G_1$ we get

$L\xi(G_1) = \xi(G_k) - 3(k+1) = 9k^2 + 9k$

Let $G_2$ be the graph



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:




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 $C_{k+2}H_{2k+6}$.

In this case, we will get an increase in the eccentricity to $\frac{1}{2}(k+1)$ of carbon vertices by two. Also will get an increase in eccentricity to $k+2$ of hydrogen vertices by 2

Thus

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

$$= (9k^2 + 9k) + (27k + 51) + \frac{1}{2}(k-1)(6)(2) + (1)(3)(2) + (k+2)(3)(2)$$

$$= 9k^2 + 48k + 63$$

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

Since the assertion is true when $n = 1$, 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

$$L\xi(G) = 9n^2 + 12n + 3, \text{ for all } n \text{ odd}, n \geq 1 \qquad \square$$

## 3 CONCLUSION

We computed a recently introduced topological invariant called LECI for some special classes of chemical trees. Also we presented some simple applications of these results, especially related such as group of alkanes. This research paves the way for future investigations in generalizing the results corresponding alkanes. Future research may address the LECI index of group of alkenes and group of alkynes.

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