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On leap eccentric connectivity index of thorny graphs

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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 $d_2(v)$. 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 thorny graphs namely, thorny complete graph, thorny complete bipartite graph, thorny cycles and thorny paths. Also we discuss some of its applications in chemical structures such as cyclo-alkanes.

KEYWORDS

Leap Zagreb indices; eccentricity; leap eccentric connectivity index.

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 thorny graphs such as thorny complete graph, thorny complete bipartite graph, thorny star graph, thorny cycles and thorny paths. Also we have discussed some applications of these results related to chemical compounds. 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 $LM_2(G)=\sum_{uv\in E(G)} d_2(u)d_2(v)\cdot$

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

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.

Definition 4. The LECI of G is defined as $L\xi^C(G)=\sum_{v\in V(G)} d_2(v)e(v)$ where $e(v)$ is the eccentricity of a vertex v in G.

Let us denote $T=\sum_{i=1}^{n} p_i$.

In this section, we study this index over some special classes of thorny graphs like thorny complete graph, thorny complete bipartite graph, thorny cycle and thorny path.

Thorny complete graph

Let K_n be a complete graph with n vertices. Then the thorny complete graph K_n^* is a graph obtained from K_n by attaching p_i thorns to every vertex v_i of K_n.

Theorem 5. $L\xi^c(K_n^*)=3\sum_{i=1}^{n} p_i^2+(5n-8)T$.

Proof:

Let $V(K_n)=\{v_1,v_2,\ldots,v_n\}$ and $V(K_n^*)=V(K_n)\cup V'$ where $V'=\{v^{ij}:1\le j\le p_i, 1\le i\le n\}$ is the set of p_i thorns attached to every vertex v_i, $1\le i\le n$. Then we can observe the following:

(i) $e(v_i)=2, 1\le i\le n$

(ii) $e(v^{ij})=3, 1\le j\le p_i, 1\le i\le n$

(iii) $d_2(v_i)=\sum_{j=1, j\ne i}^{n} p_j, 1\le i\le n$

(iv) $$\begin{aligned} d_2(v^{ij}) &= p_i-1+\deg(v_i:K_n)\\ &= p_i+n-2, 1\le j\le p_i, 1\le i\le n\end{aligned}$$

Now,

$$\begin{aligned} L\xi^c(K_n^*) &= \sum_{v\in V(K_n^*)} d_2(v)e(v)\\ &= \sum_{v\in V(K_n)} d_2(v)e(v)+\sum_{v\in V'} d_2(v)e(v)\\ &=2\sum_{i=1}^{n}\sum_{j=1, j\ne i}^{n} p_j+3\sum_{i=1}^{n}\sum_{j=1}^{p_i}(p_i+n-2)\\ &=2\sum_{i=1}^{n}(T-p_i)+3\sum_{i=1}^{n} p_i^2+3nT-6T\\ &=3\sum_{i=1}^{n} p_i^2+(5n-8)T.\end{aligned}$$

Corollary 6: For a t-thorny complete graph K_n^t, $L\xi^c(K_n^t)=(3t-5n-8)nt$.

Thorny star graph

The thorny star graph $K_{1,n}^{*}$ is shaped from a star $K_{1,n}$ by attaching a number of thorns to every vertex of $K_{1,n}$.

Theorem 7:

$$L\xi^{c}(K_{1,n}^{*}) = 2(T - p_{n+1}) + 3n)n - 1) + (6n-3)p_{n+1} + 4\sum_{i=1}^{n+1} p_i^2 - p_{n+1}^2.$$

Proof: Let $V(K_{1,n}) = \{v, v_1, v_2, ..., v_n\}$ where v is the central vertex and the remaining vertices are leaves of the star $K_{1,n}$. Then $V(K_{1,n}^{*}) = V(K_{1,n}) \cup V' \cup V''$ where $V' = \{v_i^j : 1 \le j \le p_i, 1 \le i \le n\}$ is the set of p_i thorns attached to v_i and $V'' = \{v^j : 1 \le j \le p_{n+1}\}$ is the set of p_{n+1} thorns attached to the central vertex v of $K_{1,n}$. The 2-degree and eccentricity of every vertex in $K_{1,n}^{*}$ are given in Table 1 as follows:

TABLE 1 2-Degree and eccentricity of every vertex in $K_{1,n}^{*}$

Vertex u	$d_2(u)$	$e(u)$
v	$T - p_{n+1}$	2
v_i, $1 \le i \le n$	$n - 1 + p_{n+1}$	3
$v_i^j, 1 \le j \le p_i, 1 \le i \le n$	p_i	4
$v^j, 1 \le j \le p_{n+1}$	$p_{n+1} + n - 1$	3

By the definition of LECI,

$$L\xi^{c}(K_{1,n}^{*}) = \sum_{u \in V(K_{1,n}^{*})} d_2(u)e(u)$$

$$= \sum_{u \in V(K_{1,n})} d_2(u)e(u) + \sum_{i=1}^{n}\sum_{j=1}^{p_i} d_2(v_i^j)e(v_i^j) + \sum_{j=1}^{p_{n+1}} d_2(v^j)e(v^j)$$

$$= 2(T - p_{n+1}) + 4\sum_{i=1}^{n} p_i^2 + 3\sum_{i=1}^{n}[n - 1 + p_{n+1}] + 3\sum_{j=1}^{p_{n+1}}(p_{n+1} + n - 1)$$

$$= 2(T - p_{n+1}) + 4\sum_{i=1}^{n+1} p_i^2 + 3n(n-1) + (6n-3)p_{n+1} - p_{n+1}^2.$$

Corollary 8: If we set $p_i = t$ for all $1 \le i \le p_{n+1}$, then

$$L\xi^{c}(K_{1,n}^{t}) = 3n(n-1) + (8n-5)t + (4n+3)t^2.$$

Thorny complete bipartite graph

The thorny complete bipartite graph $K_{m,n}^{*}$ is a graph obtained from a complete bipartite graph $K_{m,n}$ by attaching a number of thorns to each vertex of $K_{m,n}$.

Theorem 9. For a complete bipartite graph $K_{m,n}$, where m,n>1, let $V(K_{m,n}) = \{u_1, u_2, ..., u_m\} \cup \{v_1, v_2, ..., v_n\}$. Let p_i and $p_j^{'}$ be the number of thorns attached to u_i and v_j respectively, $1 \le i \le m, 1 \le j \le n$ to form $K_{m,n}^{*}$. Then

$$L\xi^{c}(K_{m,n}^{*}) = 3(m^2 + n^2) - 3(m+n) + (7n-4)\sum_{i=1}^{m} p_i + (7m-4)\sum_{j=1}^{n} p_j^{'} + 4\sum_{i=1}^{m} p_i^2 + 4\sum_{j=1}^{n} p_j^{'2}.$$

Proof: Let $V(K_{m,n}^{*}) = V(K_{m,n}) \cup V' \cup V''$ where $V' = \{x_i^k : 1 \le k \le p_i, 1 \le i \le m\}$ is the set of p_i thorns attached to $u_i, 1 \le i \le m$ and $V'' = \{y_j^k : 1 \le k \le p_j^{'}\}$ is the set of $p_j^{'}$ thorns attached to $v_j, 1 \le j \le n$, in $K_{m,n}^{*}$.

First, we observe 2-degree and eccentricity of every vertex in $K_{m,n}^{*}$ given in Table 2.

TABLE 2 2-degree and eccentricity of every vertex in $K_{m,n}^{*}$

Vertex u	$d_2(u)$	$e(u)$
$u_i, 1 \le i \le m$	$\sum_{j=1}^{n} p_j^{'} + (m-1)$	3
$v_j, 1 \le j \le n$	$\sum_{i=1}^{m} p_i + (n-1)$	3
$x_i^k, 1 \le k \le p_i, 1 \le i \le m$	$p_i + n - 1$	4
$y_j^k, 1 \le k \le p_j^{'}, 1 \le j \le n$	$p_j^{'} + m - 1$	4

Now, we have

$$L\xi^c(K^*_{m,n}) = \sum_{u\in V(K^*_{m,n})} d_2(u)e(u)$$

$$= \sum_{u\in V(K_{m,n})} d_2(u)e(u) + 4\sum_{i=1}^{m} p_i(p_i+n-1)$$

$$+4\sum_{j=1}^{n} p_j^{'}(p_j^{'}+m-1)$$

$$=3\sum_{i=1}^{m}\sum_{j=1}^{n}(p_j^{'}+m-1)+3\sum_{j=1}^{n}\sum_{i=1}^{m}(p_i+n-1)$$

$$+4\sum_{i=1}^{m} p_i(p_i+n-1)+4\sum_{j=1}^{n} p_j^{'}(p_j^{'}+m-1)$$

$$=3m(m-1)+3m\sum_{j=1}^{n} p_j^{'}+3n(n-1)+3n\sum_{i=1}^{m} p_i$$

$$+4\sum_{i=1}^{m} p_i^2+4(n-1)\sum_{i=1}^{m} p_i+4\sum_{j=1}^{n} p_j^{'2}$$

$$+4(m-1)\sum_{j=1}^{n} p_j^{'}.$$

Corollary 10: For a t-thorny complete bipartite graph $K^t_{m,n}$,

$$L\xi^c(K^t_{m,n}) = 3(m^2+n^2)-3(m+n)$$
$$+14mnt-4(m+n)t+4(m+n)t^2.$$

Thorny cycle graph

The thorny cycle graph C_n^* is a graph obtained from a cycle C_n of length n by attaching p_i thorns to each vertex v_i of C_n.

Theorem 11:

$$L\xi^c(C_n^*) = \begin{cases} 4\sum_{i=1}^{n} p_i^2+10T+12, \text{ if } n=4 \\ 3T\left\lfloor \frac{n}{2}\right\rfloor + \left(\left\lfloor \frac{n}{2}\right\rfloor+2\right)\sum_{i=1}^{n} p_i^2 + \\ 2n\left(\left\lfloor \frac{n}{2}\right\rfloor+1\right)+4T, \text{ if } n\geq 5. \end{cases}$$

Proof:

Let $V(C_n)=\{v_1,v_2,...,v_n\}$ & $V(C_n^*)=V(C_n)\cup V'$ where $V'=\{v_i^j : 1\leq j\leq p_i, 1\leq i\leq n\}$ is the set of p_i pendant vertices attached to $v_i, 1\leq i\leq n$.

Case 1: $n=4$

In this case, the eccentricity and 2-degree of vertices in C_n^* are given by

$e(v_i)=3, 1\leq i\leq 4$

$e(v_i^j)=4, 1\leq j\leq p_i, 1\leq i\leq 4$

$d_2(v_1)=d_2(v_3)=p_2+p_4+1$

$d_2(v_2)=d_2(v_4)=p_1+p_3+1$

$d_2(v_i^j)=p_i+1, 1\leq j\leq p_i, 1\leq i\leq 4.$

By the definition of LECI,

$$L\xi^c(C_4^*) = 3(2T+4)+4\sum_{i=1}^{4} p_i(p_i+1)$$

$$=10T+4\sum_{i=1}^{4} p_i^2+12.$$

Case 2: $n\geq 5$

One can easily observe the following:

$e(v_i)=\left\lfloor \frac{n}{2}\right\rfloor+1, 1\leq i\leq n$

$e(v_i^j)=\left\lfloor \frac{n}{2}\right\rfloor+2, 1\leq j\leq p_i, 1\leq i\leq n$

$d_2(v_1)=p_2+p_n+2$

$d_2(v_n)=p_1+p_{n-1}+2$

$d_2(v_i)=p_{i-1}+p_{i+1}+2, 2\leq i\leq n-1$

$d_2(v_i^j)=p_i+1, 1\leq j\leq p_i, 1\leq i\leq n.$

$$L\xi^c(C_n^*)=(p_2+p_n+2)\left(\left\lfloor \frac{n}{2}\right\rfloor+1\right)+(p_{n-1}+p_1+2)\left(\left\lfloor \frac{n}{2}\right\rfloor+1\right)$$
$$+\sum_{i=2}^{n-1}(p_{i-1}+p_{i+1}+2)\left(\left\lfloor \frac{n}{2}\right\rfloor+1\right)+\sum_{i=1}^{n}\sum_{j=1}^{p_i}(p_i+1)\left(\left\lfloor \frac{n}{2}\right\rfloor+2\right)$$
$$=2T\left(\left\lfloor \frac{n}{2}\right\rfloor+1\right)+2n\left(\left\lfloor \frac{n}{2}\right\rfloor+1\right)$$
$$+\left(\left\lfloor \frac{n}{2}\right\rfloor+2\right)\sum_{i=1}^{n} p_i(p_i+1).$$

Therefore,

$$L\xi^c(C_n^*)=3T\left\lfloor \frac{n}{2}\right\rfloor+\left(\left\lfloor \frac{n}{2}\right\rfloor+2\right)\sum_{i=1}^{n} p_i^2$$
$$+2n\left(\left\lfloor \frac{n}{2}\right\rfloor+1\right)+4T.$$

Corollary 12: If $p_i=t$ *for all* $1\leq i\leq n$, then

$$L\xi^c(C_n^*) = \begin{cases} 4nt^2+10nt+12, \text{when } n=4 \\ n\left\lfloor \frac{n}{2}\right\rfloor(t+1)(t+2)+2n(t+1)^2, \\ \text{when } n\geq 5. \end{cases}$$

Thorny path

The thorny path P_n^* is a graph constructed from a path P_n on n vertices by attaching p_i thorns to each of its vertices.

Theorem 13: For a thorny path P_n^*,

$$L\xi^c(P_n^*) = L\xi^c(P_n) + \sum_{i=2}^{n} p_{i-1}e(v_i) + \sum_{i=1}^{n-1} p_{i+1}e(v_i)$$
$$+ \sum_{i=1}^{n} p_i^2(e(v_i)+2) + \sum_{i=2}^{n-1} p_i e(v_i) + 2n - 4 + 4T - 3(p_1 + p_n).$$

Proof: Let the vertex set of P_n be $V(P_n) = \{v_1, v_2, ..., v_n\}$.Then $V(P_n^*) = V(P_n) \cup V'$ where $V' = \{v_{ij} : 1 \le j \le p_i, 1 \le i \le n\}$ denotes the set of p_i thorns attached to each vertex v_i, $1 \le i \le n$ of P_n to obtain P_n^*.

In order to obtain the required result we first observe the 2-degree and eccentricity of each vertex in P_n^* as follows:

(i) $d_2(v_1 : P_n^*) = d_2(v_1 : P_n) + p_2$

(ii) $d_2(v_i : P_n^*) = d_2(v_i : P_n) + p_{i-1} + p_{i+1}, \quad 2 \le i \le n-1$

(iii) $d_2(v_n : P_n^*) = d_2(v_n : P_n) + p_{n-1}$

(iv) $d_2(v_{ij}) = p_1, 1 \le j \le p_1$

(v) $d_2(v_{ij}) = p_i + 1, 1 \le j \le p_i, 2 \le i \le n-1$

(vi) $d_2(v_{nj}) = p_n, 1 \le j \le p_n$

(vii) $e(v_i : P_n^*) = e(v_i : P_n) + 1, 1 \le i \le n$

(viii) $e(v_{ij} : P_n^*) = e(v_i : P_n) + 2, 1 \le j \le p_i, \quad 1 \le i \le n$

From these observations (i) through (viii), we get

$$L\xi^c(P_n^*) = \sum_{v \in V(P_n)} d_2(v : P_n^*)e(v : P_n^*) + \sum_{v \in V'} d_2(v : P_n^*)e(v : P_n^*)$$

$$= (d_2(v_1 : P_n) + p_2)(e(v_1 : P_n) + 1)$$
$$+ \sum_{i=2}^{n-1}(d_2(v_i : P_n) + p_{i-1} + p_{i+1})(e(v_i : P_n) + 1)$$
$$+ (d_2(v_n : P_n) + p_{n-1})(e(v_n : P_n) + 1)$$
$$+ \sum_{i=1}^{n}\sum_{j=1}^{p_i} p_i(e(v_i : P_n) + 2)$$
$$= L\xi^c(P_n) + \sum_{i=1}^{n} d_2(v_i : P_n) + 2T - (p_1 + p_n)$$
$$+ \sum_{i=2}^{n} p_{i-1}e(v_i) + \sum_{i=1}^{n-1} p_{i+1}e(v_i) + 2T - 2(p_1 + p_n)$$
$$+ \sum_{i=1}^{n} p_i^2(e(v_i) + 2) + \sum_{i=2}^{n-1} p_i e(v_i)$$
$$= L\xi^c(P_n) + \sum_{i=2}^{n} p_{i-1}e(v_i) + \sum_{i=1}^{n-1} p_{i+1}e(v_i)$$
$$+ \sum_{i=1}^{n} p_i^2(e(v_i) + 2)$$
$$+ \sum_{i=2}^{n-1} p_i e(v_i) + (2n-4) + 4T - 3(p_1 + p_n).$$

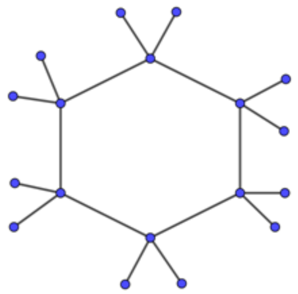

FIGURE 1 Molecular graph of Hexamethylene

Corollary 14:

$$L\xi^c(P_n^t) = L\xi^c(P_n) + 3t\sum_{i=2}^{n-1} e(v_i)$$
$$+ t^2\sum_{i=1}^{n} e(v_i) + t(e(v_1) + e(v_n))$$
$$+ 2nt^2 + (4n-6)t + 2n - 4.$$

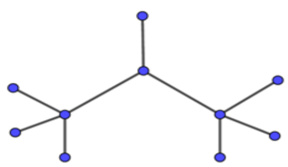

FIGURE 2 Molecular graph of Dimethylamine

Applications

In this section, we present some simple applications of the calculations that we obtained for thorny graphs.

Alkanes are chemical compounds wherein all carbon atoms are linked with single bonds. Table 3 gives the LEC index of a family of Alkanes with general formula C_nH_{2n+2} which can be computed using Theorem 13.

TABLE 3 LEC index of a family of Alkanes with general formula C_nH_{2n+2}

Alkane	Molecular Formula	LEC index
Methane	CH_4	24
Ethane	C_2H_6	66
Propane	C_3H_8	120
Butane	C_4H_{10}	198
Pentane	C_5H_{12}	288
Hexane	C_6H_{14}	402
Heptane	C_7H_{16}	528
Octane	C_8H_{18}	738
Nonane	C_9H_{20}	840
Decane	$C_{10}H_{22}$	1026

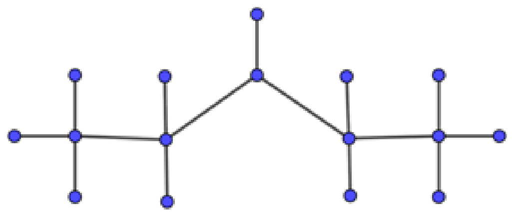

FIGURE 3 Molecular graph of Diethylamine

Table 4 gives the LECI of some simple cycloalkanes with general formula C_nH_{2n} and secondary amines.

TABLE 4 LECI of some simple cycloalkanes with general formula C_nH_{2n} and secondary amines.

Cycloalkane	Molecular Formula	LEC index
Cyclopropane (Trimethylene)	C_3H_6	78
Cyclobutane (Tetramethylene)	C_4H_8	156
Cyclopentane (Pentamethylene)	C_5H_{10}	210
Cyclohexane (Hexamethylene)	C_6H_{12}	324
Cycloheptane (Hexamethylene)	C_7H_{14}	378
Cyclooctane (Octamethylene)	C_8H_{16}	508
Cyclononane	C_9H_{18}	594
Cyclodecane	$C_{10}H_{20}$	781
Dimethylamine	$(CH_3)_2NH$	102
Diethylamine	$(CH_3CH_2)_2NH$	250

Conclusion

We computed a recently introduced topological invariant called LECI for some special classes of thorny graphs such as thorny complete graph, thorny complete bipartite graph, thorny star graph, thorny cycle and thorny path. Also we presented some simple applications of these results, especially related with thorny path and thorny cycle. This research paves the way for future investigations in generalizing the results corresponding alkanes, cycloalkanes and secondary amines. Future research may address the LECI index of isomers.

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