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FULL PAPER

Multiplicative leap Zagreb indices of T-thorny graphs

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Let G=(V, E) is a molecular graph in which the vertex set V represents atoms and the edge set E represents the bonds between the atoms, corresponding to a chemical compound. In this research study, we introduced a new type of distance based topological indices called multiplicative leap Zagreb indices which is used to analyze the structural properties of some chemicals. They are as follows $L\Pi_1(G)=\prod_{u\in V(G)} d_2(u)^2$, $L\Pi_2(G)=\prod_{uv\in E(G)} d_2(u)d_2(v)$ and $L\Pi_3(G)=\prod_{u\in V(G)} \deg(u)d_2(u)$ where $d_2(u)$ is the 2-degree of the vertex u, defined as the number of vertices which are at distance two from u in G. We computed exact values of these indices for some well known graphs and also we obtained results for a special families of t-thorny graphs namely, t-thorny path graphs, t-thorny star graphs, t-thorny complete graphs and t-thorny complete bipartite graphs and t-thorny cycles.

KEYWORDS

Zagreb indices; leap Zagreb indices; multiplicative Zagreb indices; multiplicative leap Zagreb indices; molecular graph; chemical structure.

Introduction

Drugs and other chemical compounds are often modeled as graphs called molecular graphs. Each vertex in the molecular graph represents an atom of the molecule and each edge represents the covalent bond between the atoms that are represented by edges between the corresponding atoms.

A topological index is basically a map from the set of chemical compounds represented by molecular graphs to the set of real numbers. It is the graph invariant number calculated from a graph representing a molecule. Topological indices are widely used in developing the quantitative structure-activity relationships (QSAR) in which the biological activity or other properties of molecules are correlated with their chemical structure.

One of the oldest indices in theory of chemical graphs are Zagreb indices [2] which are degree based. They are defined as follows: Let G=(V,E) be a molecular graph representing a chemical compound (possibly Hydrogen suppressed). The first Zagreb index of G is defined as $M_1(G)=\sum_{v\in V(G)} \deg(v)^2$ where deg(v) denotes the degree of a vertex v in G. The second Zagreb index of G is

$$M_2(G)=\sum_{uv\in E(G)} \deg(u)\deg(v). \qquad (1)$$

Similar to these oldest indices we have the multiplicative version of Zagreb indices in the literature namely, multiplicative Zagreb indices [1, 2, 7] of graphs including, first and second multiplicative Zagreb indices. They are defined as follows:

$$\Pi_1(G) = \prod_{v\in V(G)} \deg(v)^2 \qquad (2)$$

$$\Pi_2(G) = \prod_{uv\in E(G)} \deg(u)\deg(v). \qquad (3)$$

Recently Naji *et al.* [6] introduced a distance based topological indices called "Leap Zagreb indices" which are also known as "Zagreb connection indices" [8] in the literature. They are defined as follows:

The First leap Zagreb index of G is $LM_1(G) = \sum_{v\in V(G)} d_2(v)^2$. The second leap Zagreb index of G is $LM_2(G) = \sum_{uv\in E(G)} d_2(u)d_2(v)$ and the third leap Zagreb index of G is defined by $LM_3(G) = \sum_{v\in V(G)} \deg(v)d_2(v)$. Here $d_2(v)$ represents the 2-degree of a vertex v, which is defined as the number of vertices at distance two from v in G.

For more results about these indices one may refer [6].

We introduce a new set of topological invariants called multiplicative leap Zagreb indices of a graph G, respectively, the first, second and third multiplicative leap Zagreb indices (MLZI) and they are defined as follows:

(i) First MLZI : $L\Pi_1(G) = \prod_{v\in V(G)} d_2(v)^2$

(ii) Second MLZI: $L\Pi_2(G) = \prod_{uv\in E(G)} d_2(u)d_2(v)$

(iii) Third MLZI: $L\Pi_3(G) = \prod_{v\in V(G)} \deg(v)d_2(v)\cdot$

Results and Discussion

Multiplicative Leap Zagreb Indices of Some Well-Known Graphs

Proposition-1: For a path P_n on $n \geq 3$ vertices,

$$(i)\ L\Pi_1(G) = L\Pi_2(G) = \begin{cases} 0, when\ \ n = 3 \\ 4^{n-4}, when\ n \geq 4 \end{cases}$$

$$(ii)\ L\Pi_3(G) = \begin{cases} 0, if\ \ n = 3 \\ 4^{n-3},\ if\ \ n \geq 4. \end{cases}$$

Proposition-2: For a cycle $C_n, n \geq 3$,

$$(i)\ L\Pi_1(C_n) = L\Pi_2(C_n) = \begin{cases} 0, if\ n = 3 \\ 1, if\ n = 4 \\ 4^n, if\ n \geq 5. \end{cases}$$

$$(ii)\ L\Pi_3(C_n) = \begin{cases} 0, if\ n = 3 \\ 16, if\ n = 4 \\ 4^n, if\ n \geq 5. \end{cases}$$

On based the definitions, the proof is obvious. $L\Pi_i(G) = 0,\ i = 1,2,3$ when G is either a star graph S_n or a wheel graph $W_{1,n}$.

Proposition-3: For a complete bipartite graph $K_{r,s}, s \geq r \geq 1$,

(i) $L\Pi_1(K_{r,s}) = (r-1)^{2r}(s-1)^{2s}$

(ii) $L\Pi_2(K_{r,s}) = (r-1)^{rs}(s-1)^{rs}$

(iii) $L\Pi_{31}(K_{r,s}) = r^s s^r (r-1)^r (s-1)^s$

One can easily verify the above results by means of the following vertex and edge partitions of $K_{r,s}$.

TABLE 1 Vertex Partition

2-deg	**#**	**deg**	**#**	**v with** $(\deg(v), d_2(v))$	**#**
(r-1)	*r*	*(r-1)*	*rs*	*(r,s-1)*	*s*
(s-1)	*s*	*(s-1)*	*rs*	*(s,r-1)*	*r*

TABLE 2 Edge partition

Edge uv with 2-degree	**#edges**
(r-1,s-1)	*rs*
(s-1)	*s*

A double star D(r, s) is the graph obtained by joining the centre of two stars $K_{1,r}$ and $K_{1,s}$ with an edge.

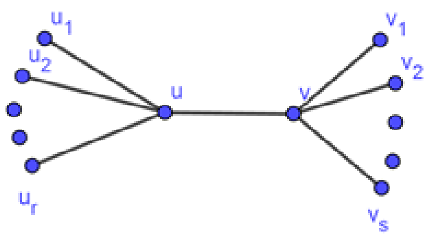

FIGURE 1 D(r,s)

Proposition-4: For a double star D(r,s) with $s \geq r \geq 1$,

(i) $L\Pi_1(D(r,s)) = \mathrm{r}^{2(\mathrm{r}+1)}\mathrm{s}^{2(\mathrm{s}+1)}$

(ii) $L\Pi_2(D(r,s)) = (\mathrm{rs})^{(\mathrm{r}+\mathrm{s}+1)}$

(iii) $L\Pi_3(D(r,s)) = \mathrm{r}^{(\mathrm{r}+1)}\mathrm{s}^{(\mathrm{s}+1)}(\mathrm{r}+1)(\mathrm{s}+1)$

Proof: It is enough to observe the vertex and edge partitions of D(r,s) with respect to 2-degree and degree of every vertex in D(r,s). The rest will follow easily from the definition of multiplicative leap Zagreb indices.

TABLE 3 Vertex partition of D(r,s)

2-deg	#	deg	#	v with $(\deg(v), d_2(v))$	#
r	(r+1)	1	(r+s)	(1,r)	r
s	(s+1)	(r+1)	1	((r+1),r)	1
		(s+1)	1	(1,s)	s
				((s+1),s)	1

TABLE 4 Edge partition of D(r, s)

Edge uv with 2-degree	# edges
(r,s)	*(r+s+1)*

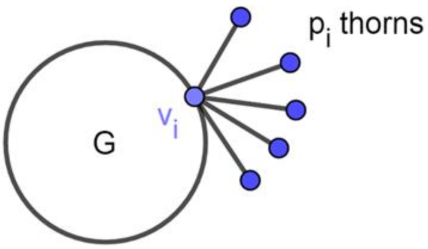

FIGURE 1 Thorny graph G*

Multiplicative leap Zagreb indices of some special classes of thorny graphs

Gutman [4] introduced the following special type of chemical graph known as thorny graph.

Let G be a simple connected graph and $\{v_1, v_2, \ldots, v_n\}$ and $\{p_1, p_2, \ldots, p_n\}$ be two sequences 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 to each vertex v_i of G. In particular, if all $p_i = t$, then we get a t-thorny graph denoted by G^t.

Hereafter we call a pendant vertex (i.e a vertex of degree 1) by a thorn.

T-thorny path graph P_n^t

The t-thorny path graph P_n^t is a graph obtained from a path P_n on n vertices by attaching t thorns to every vertex of P_n.

Theorem 1. For a t-thorny path graph P_n^t,

$$(i)\ L\Pi_1(P_n^t) = \begin{cases} t^{4(t+1)}, if\ n=2 \\ 4(t+1)^{2t+4}, if\ n=3 \\ t^{4t}(2t+1)^4(2t+2)^{2(n-4)} \\ (t+1)^{(2n-4)t+4},\ if\ n \geq 4. \end{cases}$$

$$(ii)\ L\Pi_2(P_n^t) = \begin{cases} t^{2(2t+1)}, if\ n=2 \\ t^{2t}(t+1)^{3t+2}(2t)^{t+2}, if\ n=3 \\ t^{2t}(t+1)^{nt+2}(2t+1)^{2t+4} \\ (2t+2)^{(n-4)t+2(n-4)}, if\ n \geq 4. \end{cases}$$

$$(iii)\ L\Pi_3(P_n^t) = \begin{cases} t^{2(t+1)}(t+1)^2, if\ n=2 \\ 2t^{2t+1}(t+1)^{t+4}(t+2), if\ n=3 \\ t^{2t}(t+1)^{(n-2)t+4}(t+2)^{n-2}(2t+1)^2 \\ (2t+2)^{(n-4)}, if\ n \geq 4. \end{cases}$$

Proof: Let us observe the vertex and edge partitions of P_n^t to prove this result.

TABLE 5 Vertex partition of P_n^t w.r.to 2-degree

n	2-degree	# vertices
2	*t*	*2t+2*
	t	*2t*
3	*t+1*	*t+2*
	2t	*1*
	t	*2t*
$n \geq 4$	*t+1*	*(n-2)t+2*
	2t+1	*2*
	2t+2	*n-4*

TABLE 6 Vertex partition of P_n^t w.r.to degree.

Degree	#vertices
1	nt
t+1	2
t+2	n-2

TABLE 7 Edge partition of P_n^t w.r.to 2-degree.

n	Edge uv with $(d_2(u), d_2(v))$	#edges
2	(t,t)	2t+1
3	(t,t+1)	2t
	(t+1,2t)	t+2
≥ 4	(t,t+1)	2t
	(t+1,2t+1)	2t+2
	(t+1,2t+2)	(n-4)t
	(2t+1,2t+2)	2
	(2t+2,2t+2)	n-5

The proofs of (i), (ii) and (iii) follow easily from Tables 6, 7, and 8, respectively.
For the sake of completeness, let us discuss the proof of (i) when $n \geq 4$.
By the very definition of first MLZI, we get

TABLE 8 Vertex partition of P_n^t w.r.to degree and 2-degree

n	Vertex v with $(\deg(v), d_2(v))$	#vertices
2	(1,t)	2t
	(t,t+1)	2
3	(1,t)	2t
	(1,t+1)	t
	(t+1,t+1)	2
	(t+2,2t)	1
≥ 4	(1,t)	2t
	(1,t+1)	(n-2)t
	(t+1,t+1)	2
	(t+2,2t+1)	2
	(t+2,2t+2)	n-4

$$L\Pi_1(P_n^t) = \prod_{v \in V(P_n^t)} d_2(v)^2$$
$$= [(t^{2t})^2 (t+1)^{2(2+(n-2)t)} (2t+1)^4 (2t+2)^{2(n-4)}]$$
$$= [t^{4t} (2t+1)^4 (2t+2)^{2(n-4)} \ (t+1)^{(2n-4)t+4}].$$

t-Thorny star graph S_{n+1}^t

A t-thorny star graph S_{n+1}^t is a graph obtained from a star S_{n+1} with (n+1) vertices by attaching t thorns to every vertex of S_{n+1}.

Theorem 2: For a t-thorny star graph S_{n+1}^t,

(i) $L\Pi_1(S_{n+1}^t) = t^{2nt} (nt)^2 (n-1+t)^{2(n+t)}$

(ii) $L\Pi_2(S_{n+1}^t) = t^{nt} (nt)^{n+t} (n-1+t)^{n(t+1)+t}$

(iii) $L\Pi_3(S_{n+1}^t) = t^{nt+1} (t+1)^n n(t+n)(n-1+t)^{(n+t)}$

Proof: The vertex and edge partitions of S_{n+1}^t are obtained as follows:

TABLE 9 Vertex partition of S_{n+1}^t based on 2-degree

2-degree	#vertices
t	nt
(n-1+t)	n+t
nt	1

TABLE 10 Vertex partition of S_{n+1}^t based on degree

degree	#vertices
1	nt+t
t+1	n
n+1	1

TABLE 11 Edge partition of S_{n+1}^t

Edge uv with $(d_2(u), d_2(v))$	#edges
(t,n-1+t)	nt
(n-1+t,nt)	n+t

TABLE 12 Vertex partition of S_{n+1}^t based on both degree and 2-degree

Vertex v with $(\deg(v), d_2(v))$	#vertic1es
(1,t)	nt
(t+1,n-1+t)	n
(t+n,nt)	1
(1,n-1+t)	t

For the sake of brevity, let us prove (iii) with reference to Table 12.

$$L\Pi_3(S_{n+1}^t)=\prod_v \deg(v)d_2(v)$$
$$=t^{nt}[(t+1)(n-1+t)]^n[(t+n)nt](n-1+t)^t$$
$$=t^{nt+1}(t+1)^n n(t+n)(n-1+t)^{(n+t)}$$

Similarly one can prove the remaining cases with reference to Tables 10 and 11.

T-thorny complete graph K_n^t

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

Theorem 3. For a t-thorny complete graph K_n^t,

(i) $L\Pi_1(K_n^t)=(t+n-1)^{2nt}[(n-1)t]^{2n}$

(ii) $L\Pi_2(K_n^t)=(t+n-2)^{nt}[(n-1)t]^{n(t+n-1)}$

(iii) $L\Pi_3(K_n^t)=(t+n-2)^{nt}(t+n-1)^n[(n-1)t]^n$

T-thorny complete bipartite graph $K_{r,s}^t$

The t-thorny complete bipartite graph $K_{r,s}^t$ is a graph obtained from a complete bipartite graphs $K_{r,s}$ by attaching t thorns to its each vertex.

Theorem 4. For a t-thorny complete bipartite graph $K_{r,s}^t$,

(i) $L\Pi_1(K_{r,s}^t)=[(t+s-1)^{2tr}(t+r-1)^{2ts}(rt+s-1)^{2s}(st+r-1)^{2r}]$

(ii) $L\Pi_2(K_{r,s}^t)=[(t+s-1)^{tr}(t+r-1)^{ts}(rt+s-1)^{s(t+r)}(st+r-1)^{r(t+s)}]$

(iii) $L\Pi_3(K_{r,s}^t)=[(t+s-1)^{tr}(t+r-1)^{ts}(rt+s-1)^{s}(st+r-1)^{r}(t+r)^s(t+s)^r]$

The proof of this result is similar to that of Theorem 3.

T-thorny cycle graph C_n^t

where C_n is a cycle on n vertices. Then the t-thorny cycle C_n^t is a graph obtained from C_n by attaching t thorns to every vertex of C_n.

The following Theorem gives the multiplicative leap Zagreb indices of t-thorny cycle C_n^t.

Theorem 5:

$$(i)\ L\Pi_1(C_n^t)=\begin{cases}(t+1)^{6t}(2t)^6, if\ n=3\\(t+1)^{8t}(2t+1)^8, if\ n=4\\(t+1)^{2nt}(2t+2)^{2n}, if\ n\geq 5\end{cases}$$

$$(ii)\ L\Pi_2(C_n^t)=\begin{cases}(t+1)^{3t}(2t)^{3t+6}, if\ n=3\\(t+1)^{4t}(2t+1)^{4t+8}, if\ n=4\\(t+1)^{nt}(2t+2)^{n(t+2)}, if\ n\geq 5\end{cases}$$

$$(iii)\ L\Pi_3(C_n^t)=\begin{cases}(t+1)^{3t}(t+2)^3 8t^3, if\ n=3\\(t+1)^{4t}(t+2)^4(2t+1)^4, if\ n=4\\(t+1)^{nt}(t+2)^n(2t+2)^n, if\ n\geq 5\end{cases}$$

Proof: The proof of this result is evident from the following vertex and edge partitions of C_n^t

TABLE 13 Vertex partition of C_n^t based on 2-degree

n	2-degree	#vertices
3	*t+1*	*3t*
	2t	*3*
4	*t+1*	*4t*
	2t+1	*4*
$n\geq 5$	*t+1*	*nt*
	2t+2	*n*

TABLE 14 Vertex partition of C_n^t based on degree

Degree	#vertices
1	*nt*
t+2	*n*

TABLE 15 Edge partition of C_n^t

n	Edge uv with $(d_2(u),d_2(v))$	#edges
3	*(t+1,2t)*	*3t*
	(2t,2t)	*3*

4	*(t+1,2t+1)*	*4t*
	(2t+1,2t+1)	*4*
$n \geq 5$	*(t+1,2t+2)*	*nt*
	(2t+2,2t+2)	*n*

TABLE 16 Vertex partitions of C_n^t w.r.to degree and 2-degree

n	Vertex v with (deg(v),d₂(v))	#vertices
3	*(1,t+1)*	*3t*
	(t+2,2t)	*3*
4	*(1,t+1)*	*4t*
	(t+2,2t+1)	*4*
$n \geq 5$	*(1,t+1)*	*nt*
	(t+2,2t+2)	*n*

Conclusion

In this study, a new topological invariant called multiplicative leap Zagreb indices were evaluated over some special classes of important chemical graph structure known as t-thorny graphs. It is of a great importance to study these indices over thorny graphs as well as generalized thorny graphs; especially computation of these indices for generalized thorny graphs would be a challenging one.

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