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REFORMULATED ZAGREB INDICES OF THORNY GRAPHS AND ALGORITHMS

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Abstract. Molecular descriptors (graph indices) numerically describe the topologies of the chemicals. Graph indices are used to estimate certain properties of molecules. In this paper, reformulated first/second Zagreb indices for the thorny graph of any graph are obtained. Exact results are given for the reformulated Zagreb indices of thorny graphs of some special graphs. Reformulated Zagreb indices of the propyl ether imine (PETIM) dendrimers calculated and these indices are compared numerically. In addition, algorithms are designed to calculate the reformulated first/second Zagreb indices of graphs.

1. Introduction

In recent years, due to the increase in diseases, there has been a focus on discovering new drugs. For this, scientists study topological indices to obtain information about the bioactivity and physicochemical properties of drugs (chemical structures) in a short time without conducting experiments. Graph indices are descriptors with numerical values of molecular graphs. Molecular graphs are the representation of the skeletons of chemicals with graph theory. The vertices (edges) on the graph are the atoms (bonds) of the molecule that do not contain hydrogen. Graph indices are used in quantitative structure property/activity relationship studies [9].

The first known index is the Wiener index [28]. This index depends on the distance in graph. The most studied indices are those based on the degree of the vertex, which are also easy to calculate. Gutman et al. introduced [11] the first Zagreb index of a Γ graph as

$$M_1(\Gamma) = \sum_{u\in V(\Gamma)} d(u)^2 \tag{1.1}$$

and second Zagreb index is defined as

$$M_2(\Gamma) = \sum_{uv\in E(\Gamma)} d(u)d(v) \tag{1.2}$$

where $V(\Gamma)$ is vertex set, $E(\Gamma)$ is edge set of Γ graph and $d(u)$ is degree of u vertex.

Milicevic\`et al. introduced the edge version of these indices [19]. These indices are called reformulated Zagreb indices (RZI) and are defined as

$$RM_1(\Gamma) = \sum_{e\in E(\Gamma)} d(e)^2, \tag{1.3}$$

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$$RM_2(\Gamma) = \sum_{e \sim f} d(e)d(f) \tag{1.4}$$

where $d(e)$ is degree of e edge and e is adjacent to the edge f, denoted as $e \sim f$. Recently, Stankov et al. obtained relations between reformulated Zagreb indices and coindices [27]. Pattabiriman and Santhakumar obtained reformulated Zagreb indices for F-sum of graphs [23]. Maji et al. studied inverse problem for reformulated first Zagreb index [18]. Liu et al. derived expressions for these indices of some graphs [17]. Colakoglu found some result on RZI of cycle-related and linear phenylenes graphs [5]. Naureen et al. studied the enthalpy of benzenoid hydrocarbons and molecular trees with general multiplicative Zagreb indices [22]. Rao et al. performed QSPR analysis of cactus type graphs based on Zagreb indices [25].

Thorny graph is obtained from graph Γ by attaching p_i new vertices degree to one each v_i vertex of a Γ graph for p_i non-negative integers $i = 1, 2, \ldots, n$ [10]. Caterpillars known as Gutman trees are thorny tree graphs. These graphs have been studied for benzenoid hydrocarbons in chemical graph theory [8]. The thorny star and double star (bistar) graphs are also thorny tree graphs. These graphs correspond to the chemical graph structure of dendrimers. Figure 1 shows a tree graph, Γ with 21 vertices and its thorny graph with $p_1 = 2, p_3 = 1, p_6 = 5, p_8 = 1, p_{11} = 3, p_{15} = 2, p_{16} = 1, p_{21} = 2$, $p_i = 0$ for $2 \leq i \leq 20$ when $i \neq 3, 6, 8, 11, 15, 16, 21$. Here, the new edges added with dashed lines are the elements of the E$'$ set of the thorny graph, Γ^*. For example, $d\left(v_1\right) = 5, d_{v_1}^* = 5 + p_1 = 7, d\left(v_8\right) = 1, d_{(v_8)}^* = 1 + p_8 = 2, d_e = 4, d_{e^*} = d(e) + p_i + p_j = 4 + 2 + 1 = 7$ for $e^* = v_1 v_8 = e \in E(\Gamma), d(f) = d\left(v_8\right) + p_8 - 1 = 1$ for $e^* \in E', v_8 \in V(\Gamma)$.

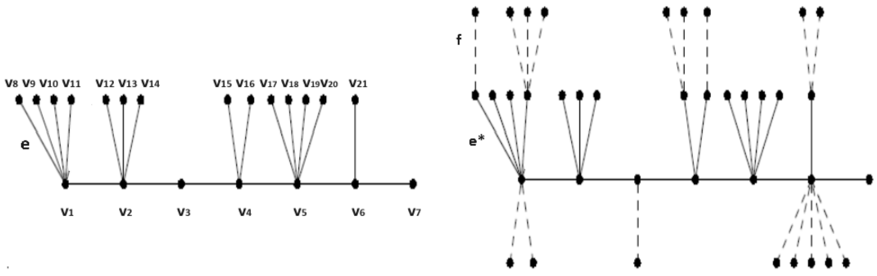

Figure 1. A tree graph, Γ and its thorny graph, Γ^*.

Schmuck et al. studied Wiener-type indices for greedy tree and caterpillar [26]. Jalali et al. calculated some Zagreb indices of thorny graphs [14]. Idrees et al. computed degree-based indices for thorny graphs of some special graphs [13]. Natarajan et al. studied the forgotten index of thorny graphs [21]. In the literature, there are many studies on thorny graphs and topological indices (See details [3],[6],[7],[12]).

In this study, bounds are obtained for the reformulated Zagreb indices of the thorny graph. Exact values for reformulated Zagreb indices of double star graph and Caterpillar which are thorny graphs, and also thorny cycle are given. Algorithms are given to calculate reformulated Zagreb indices of any graph. The reformulated first and second Zagreb indices of the propyl ether imine dendrimers are calculated and these two results are compared numerically.

2. Preliminaries

Let $\Gamma(V(\Gamma), E(\Gamma))$ be a graph. The degree of an edge e is represent by $d(e)$ [4]. In this section, information about some special thorny graphs will be given.

Definition 2.1. Assume that $K_{1,n}$ is star graph whit $n+1$ vertices. Let vertices of $K_{1,n}$ be labeled as v_i, $i = 1, 2, ..., n$ and central vertex of star graph be labeled as v_c. Thorny star graph, $K^*_{1,n}$ is obtained by adding p_c thorns to v_c and p_i thorns to each v_i vertex of $K_{1,n}$ [10].

Definition 2.2. The double star graph, $D_{r,s}$, is obtained by joining the central vertices of two-star graph whit r vertices and s vertices with an edge. This graph has $r + s + 2$ vertices and $r + s + 1$ edges [10]. Figure 2 shows double star graph, $D_{3,5}$, with $3 + 5 + 2 = 10$ vertices.

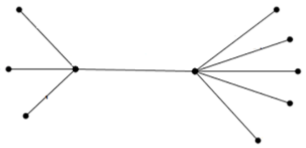

Figure 2. Double star graph, $D_{3,5}$

Definition 2.3. The caterpillar has a central path graph and leaves. Let $T(p_1, p_2, ..., p_i)$ for $i = 1, 2, ..., r$ be a caterpillar whose center is the path graph P_r Assume that p_i is the number of leaves at the ith vertex of the central path graph, P_r If the degrees of each vertex of the caterpillar are equal, this graph is called a regular graph. The cardinality of vertex set, n is equal to and the cardinality of edge set, m, is equal to $n - 1$ [10]. Figure 3 shows a caterpillar with $p_i = 3, i = 1, 2, ..., r$.

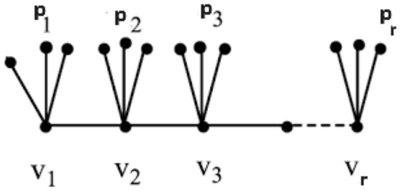

Figure 3. Caterpillar graph, $T(3, 3, ..., 3)$

Definition 2.4. Assume that C_n is a cycle graph with n vertices and vertices of C_n are labeled as v_i, $i = 1, 2, ..., n$ Thorny cycle graph, C^*_n , is obtained by adding p_i thorns to each v_i vertex of C_n [10].

3. Reformulated Zagreb Indices of Thorny Graphs

In this section, it is obtained RZI of any Γ graph. Then, exact formulas for RZI of special graphs such as double star graph, Caterpillar, thorny cycle, and thorny star graphs are obtained.

Theorem 3.1. *Let Γ be any graph with n vertices Then*

$$RM_1(\Gamma^*) \le \left(\sqrt{RM_1(\Gamma)} + \sqrt{\theta(\Gamma)}\right)^2 + \left(\sqrt{M_1(\Gamma)} + \sqrt{\phi(\Gamma)}\right)^2$$

where $\theta(\Gamma) = \sum_{v_i v_j \in E(\Gamma)} (p_i + p_j)^2$ *and* $\phi(\Gamma) = \sum_{v_i \in V(\Gamma)} (p_i - 1)^2$.

Proof. Let vertices of Γ be labelled as $v_i, i = 1, 2, \ldots, n$, and Γ^* be thorny graph of Γ. The edge set of Γ^* is equal to $\mathrm{E}^* = E(\Gamma) \cup E'$ where E' is set of pendent edges. Then,

$$RM_1(\Gamma^*) = \sum_{e^* \in E^*} d(e^*)^2 = \sum_{e^* \in E(\Gamma)} d(e^*)^2 + \sum_{e^* \in E'} d(e^*)^2 . \tag{3.1}$$

It is easy to see that $d(e^*) = d(e) + p_i + p_j$ for $e^* = v_i v_j = e \in E(\Gamma)$ and $d(e^*) = d(v_i) + p_i - 1$ for $e^* \in E', v_i \in V(\Gamma)$ (See Figure 1). So, the equation (3.1) can be rewritten as

$$RM_1(\Gamma^*) = \sum_{v_i v_j \in E(\Gamma)} \left(d(v_i v_j) + p_i + p_j\right)^2 + \sum_{v_i \in V(\Gamma)} \left(d(v_i) + p_i - 1\right)^2$$

or

$$\begin{aligned} RM_1(\Gamma^*) = &\sum_{v_i v_j \in E(\Gamma)} d(v_i v_j)^2 + \sum_{v_i v_j \in E(\Gamma)} (p_i + p_j)^2 + 2 \sum_{v_i v_j \in E(\Gamma)} d(v_i v_j)(p_i + p_j) \\ &+ \sum_{v_i \in V(\Gamma)} d(v_i)^2 + \sum_{v_i \in V(\Gamma)} (p_i - 1)^2 + 2 \sum_{v_i \in V(\Gamma)} d(v_i)(p_i - 1) . \end{aligned}$$

From the Cauchy-Schwarz inequality, the following inequality is obtained:

$$\begin{aligned} RM_1(\Gamma^*) \leq &\sum_{e \in E(\Gamma)} d(e)^2 + \sum_{v_i v_j \in E(\Gamma)} (p_i + p_j)^2 + 2 \sqrt{\sum_{e \in E(\Gamma)} d(e)^2} \sqrt{\sum_{v_i v_j \in E(\Gamma)} (p_i + p_j)^2} \\ &+ \sum_{v_i \in V(\Gamma)} d(v_i)^2 + \sum_{v_i \in V(\Gamma)} (p_i - 1)^2 \\ &+ 2 \sqrt{\sum_{v_i \in V(\Gamma)} d(v_i)^2} \sqrt{\sum_{v_i \in V(\Gamma)} (p_i - 1)^2}. \end{aligned}$$

From the equation (1.1) and (1.3), the proof is completed. $\square$

Corollary 3.2. *Let Γ be any graph with n vertices and m edges. If $p_i = p$ for $v_i \in V(\Gamma)$ then*

$$RM_1(\Gamma^*) \leq \left(\sqrt{RM_1(\Gamma)} + 2p\sqrt{m}\right)^2 + \left(\sqrt{M_1(\Gamma)} + (p-1)\sqrt{n}\right)^2 .$$

Theorem 3.3. *Let Γ be any graph with n vertices. Then*

$$\begin{aligned} \mathrm{RM}_2(\Gamma^*) \leq &\left(\sqrt{RM_1(\Gamma)} + \sqrt{\theta(\Gamma)}\right)\left(\sqrt{RM_1(\Gamma)} + \sqrt{\theta(\Gamma)} + \sqrt{M_1(\Gamma)} + \sqrt{\phi(\Gamma)}\right) \\ &+ \sum_{v_i \in V(\Gamma)} \left(\frac{p_i(p_i - 1)}{2}\right)\left(d(v_i) + p_i - 1\right)^2 \end{aligned}$$

where

$$\theta(\Gamma) = \sum_{v_i v_j \in E(\Gamma)} (p_i + p_j)^2 \quad \text{and} \quad \phi(\Gamma) = \sum_{v_i \in V(\Gamma)} (p_i - 1)^2 .$$

Proof. Let vertices of Γ be labelled as $v_i, i = 1, 2, \ldots, n$, and Γ^* be thorny graph of Γ. The edge set of Γ^* is equal to $E^* = E(\Gamma) \cup E'$ where E' is set of pendent edges. Let $e \sim f$ for $v_i v_j = e$ and $v_j v_k = f$.

Then,

$$\begin{aligned} RM_2\left(\Gamma^*\right) &= \sum_{\substack{e,f\in E^* \\ e\sim f}} d(e)d(f) \qquad (3.2)\\ &= \sum_{\substack{e,f\in E(\Gamma) \\ e\sim f}} d(e)d(f) + \sum_{\substack{e\in E(\Gamma), f\in E' \\ e\sim f}} d(e)d(f) + \sum_{\substack{e,f\in E' \\ e\sim f}} d(e)d(f). \end{aligned}$$

It is known that $d\left(e^*\right) = d(e) + p_i + p_j$ for $e^* = v_iv_j = e \in E(\Gamma)$ and $d\left(e^*\right) = d\left(v_i\right) + p_i - 1$ for $e^* \in E', v_i \in V(\Gamma)$. So, the equation (3.2) can be rewritten as

$$\begin{aligned} RM_2\left(\Gamma^*\right) = &\sum_{e\sim f\in E(\Gamma)} \left(d(e)+p_i+p_j\right)\left(d(f)+p_i+p_j\right)\\ &+ \sum_{e\in E(\Gamma), f\in E'} \left(d(e)+p_i+p_j\right)\left(d\left(v_i\right)+p_i-1\right)\\ &+ \sum_{e\sim f\in E'} \left(d\left(v_i\right)+p_i-1\right)\left(d\left(v_i\right)+p_i-1\right). \end{aligned}$$

From the Cauchy-Schwarz inequality,

$$\begin{aligned} RM_2\left(\Gamma^*\right) \leq &\sqrt{\sum_{e\in E(\Gamma)} \left(d(e)+p_i+p_j\right)^2} \left(\sqrt{\sum_{f\in E(\Gamma)} \left(d(f)+p_j+p_k\right)^2} + \sqrt{\sum_{v_j\in V(\Gamma)} \left(d\left(v_j\right)+p_j-1\right)^2} \right) \qquad (3.3)\\ &+ \sum_{v_i\in V(\Gamma)} \left(\frac{p_i\left(p_i-1\right)}{2}\right)\left(d\left(v_i\right)+p_i-1\right)^2. \end{aligned}$$

It is clear that

$$\sum_{e\in E(\Gamma)} \left(d(e)+p_i+p_j\right)^2 \leq \left(\sqrt{\sum_{e\in E(\Gamma)} d(e)^2} + \sqrt{\sum_{e\in E(\Gamma)} \left(p_i+p_j\right)^2} \right)^2. \qquad (3.4)$$

The equation (3.3) can be rewritten using the equation (3.4) as follow

$$\begin{aligned} RM_2\left(\Gamma^*\right) \leq &\left(\sqrt{\sum_{e\in E(\Gamma)} d(e)^2} + \sqrt{\sum_{e\in E(\Gamma)} \left(p_i+p_j\right)^2} \right) \times\\ &\times \left(\sqrt{\sum_{f\in E(\Gamma)} d(f)^2} + \sqrt{\sum_{f\in E(\Gamma)} \left(p_j+p_k\right)^2} + \sqrt{\sum_{v_j\in V(\Gamma)} d\left(v_j\right)^2} + \sqrt{\sum_{v_j\in V(\Gamma)} \left(p_j-1\right)^2} \right)\\ &+ \sum_{v_i\in V(\Gamma)} \left(\frac{p_i\left(p_i-1\right)}{2}\right)\left(d\left(v_i\right)+p_i-1\right)^2. \end{aligned}$$

From the equation (1.1) and (1.3), the proof is completed. □

Theorem 3.4. *Let $K_{1,n}^*$ be thorny star graph. Then,*

$$RM_1\left(K_{1,n}^*\right) = \sum_{i=1}^{n} p_i^3 + \sum_{i=1}^{n} \left(p_i+p_c+n-1\right)^2 + p_c\left(p_c+n-2\right)^2.$$

Proof. Let $K_{1,n}^{*}$ be thorn star graph obtained from p_i attaching to each v_i of $K_{1,n}$. Let v_c be a central vertex of the star graph and p_c be thorn(s) attaching to v_c. Table 1 shows the edge partitions of the thorn star graph from the Definition 2.1.

TABLE 1. The partitions of a thorny star graph

$Frequency$	$\boldsymbol{d(e)\text{fore}\in E\left(K_{1,n}^{*}\right)}$
p_i	$p_i\text{for}1\leq i\leq n$
1	$p_i+p_c+n-1\text{for}1\leq i\leq n$
p_c	p_c+n-2

From Eq.(1.3) and Table 1, the proof is completed. □

Corollary 3.5. *Let* Γ^{*} *be the thorn star graph obtained by attaching* p *thorn to each* v_i *vertex of* $K_{1,n}$ *star graph. Then,*

$$RM_1\left(\Gamma^{*}\right)=np^{3}+n(2p+n-1)^{2}+p(p+n-1)^{2}.$$

Theorem 3.6. *Let* $K_{1,n}^{*}$ *be thorny star graph. Then,*

$$\begin{aligned} RM_2\left(K_{1,n}^{*}\right)=&\sum_{i=1}^{n}\sum_{j=1}^{p_i-1}p_i^{2}\left(p_i-j\right)+\sum_{i=1}^{n}p_i^{2}(p_i+p_c+n-1)\\ &+\sum_{i=1}^{n-1}\left(p_i+p_c+n-1\right)\left(p_{i+1}+p_c+n-1\right)\\ &+\sum_{j=1}^{p_c-1}\left(p_c-j\right)\left(p_c+n-2\right)^{2}+p_c\sum_{i=1}^{n}\left(p_c+n-2\right)\left(p_i+p_c+n-1\right). \end{aligned}$$

Proof. Let $K_{1,n}^{*}$ be thorn star graph obtained from p_i attaching to each v_i of $K_{1,n}$. Let v_c be a central vertex of the star graph and p_c be thorn(s) attaching to v_c. Table 2 shows edge degree partitions of the thorn star graph.

TABLE 2. Frequency of graph according to edge degrees of a thorny star graph

:

$Frequency$	$\boldsymbol{(d(e),d(f))fore\sim f\in E\left(K_{1,n}^{*}\right)}$
$1\leq j\leq p_i-1,(p_i-j)$	$(p_i,p_i)\,for1\leq i\leq n$
p_i	$(p_i,p_i+p_c+n-1)\,for1\leq i\leq n$
1	$(p_i+p_c+n-1,p_{i+1}+p_c+n-1)$ for $1\leq i\leq n-1$
$(p_c-j),1\leq j\leq p_c-1$	(p_c+n-2,p_c+n-2)
p_c	$(p_c+n-2,p_i+p_c+n-1)\,for1\leq i\leq n$

From Eq.(1.4) and Table 2, the proof is completed. □

Corollary 3.7. *Let Γ^* be the thorn star graph obtained by attaching p thorn to each v_i vertex of $K_{1,n}$ star graph. Then,*

$$RM_2\left(\Gamma^*\right)=n\left(\frac{p^3(p+1)}{2}+(p+n-1)\left(3p^2+p(n-1)\right)+(2p+n-1)^2\right).$$

Theorem 3.8. *Let $D_{r,s}$ be double star graph with $r+s+2$ vertices. Then*

$$RM_1\left(D_{r,s}\right)=r^3+s^3+(r+s)^2.$$

Proof. Let $S_{1,r}$ and $S_{1,s}$ be star graphs with $r+1$ and $s+1$ vertices, respectively. From the Definition 2.2, the double star graph has edge partitions in Table 3.

TABLE 3. Frequency of graph according to edge degrees of a double star graph

$Frequency$	$\boldsymbol{d}(\boldsymbol{e}) for \boldsymbol{e} \in \boldsymbol{E}\left(\boldsymbol{D}_{r,s}\right)$
r	r
s	s
1	$r+s$

From Eq.(1.3) and Table 3, the proof is completed. □

Corollary 3.9. *Let $D_{r,r}$ be double star obtained from two-star graph with $r+1$ vertices. Then,*

$$RM_1\left(D_{r,r}\right)=2r^3+4r^2.$$

Theorem 3.10. *Let $D_{r,s}$ be double star graph with $r+s+2$ vertices. Then*

$$RM_2\left(D_{r,s}\right)=\frac{r^3(r+1)}{2}+\frac{s^3(s+1)}{2}+\left(r^2+s^2\right)(r+s).$$

Proof. Table 4 shows the degree of edges for the double star graph.

TABLE 4. The degree of edges for the double star graph

$Frequency$	$(\boldsymbol{d}(\boldsymbol{e}), \boldsymbol{d}(\boldsymbol{f})) for \boldsymbol{e} \sim \boldsymbol{f} \in \boldsymbol{E}\left(\boldsymbol{D}_{r,s}\right)$
$\frac{r(r-1)}{2}$	(r,r)
$\frac{s(s-1)}{2}$	(s,s)
r	$(r,r+s)$
s	$(s,r+s)$

From Eq. (1.4) and Table 4, the proof is completed. □

Corollary 3.11. *Let $D_{r,r}$ be with $2r+2$ vertices. Then,*

$$RM_2\left(D_{r,r}\right)=r^3(r+5).$$

Theorem 3.12. *Let Γ be caterpillar $T_n\left(p_1, p_2, \ldots, p_{r-1}, p_r\right)$ with n vertices. Then*

$$RM_1(\Gamma) = p_1^3 + p_r^3 + \sum_{i=2}^{r-1} p_i\left(p_i+1\right)^2 + \left(p_1+p_2+1\right)^2 + \left(p_{r-1}+p_r+1\right)^2 + \sum_{i=2}^{r-2}\left(p_i+p_{i+1}+2\right)^2.$$

Proof. Let the vertices of central path P_r in Γ be labeled as $v_i, i = 1, 2, \ldots, r$. The degrees of the vertices with v_1 and v_r are p_1+1 and p_r+1, respectively. The degrees of the other vertices in the central path graph are p_i+2 for $i = 2, \ldots, r-1$. Then, the degrees of the edge of caterpillar are shown in Table 5. From Eq. (1.3) and Table 5, the proof is completed.

TABLE 5. The edges of caterpillar

Frequency	$\boldsymbol{d(e)}$
p_1	p_1
p_i	$p_i+1 \quad for 2 \le i \le r-1$
p_r	p_r
1	p_1+p_2+1
1	$p_{r-1}+p_r+1$
1	$p_i+p_{i+1}+2 \quad for 2 \le i \le r-2$

□

Corollary 3.13. *Let Γ be caterpillar $T_n(p, p, \ldots, p)$ with n vertices and P_r central path graph. Then*

$$RM_1(\Gamma) = 2p^3 + 2(2p+1)^2 + (p+1)^2(p(r-2) + 4(r-3)).$$

Theorem 3.14. *Let Γ be caterpillar $T_n\left(p_1, p_2, \ldots, p_{r-1}, p_r\right)$ with n vertices. Then*

$$\begin{aligned} RM_2(\Gamma) = & \frac{p_1^3\left(p_1-1\right)}{2} + \frac{p_r^3\left(p_r-1\right)}{2} + \left(p_1+p_2+1\right)\left[\left(p_2+1\right)^2 + p_1^2 + p_3\right] \\ & + \sum_{i=2}^{r-2} p_i\left(p_i+1\right)\left(p_i+p_{i+1}+2\right) + \sum_{i=2}^{r-1} \frac{p_i\left(p_i-1\right)}{2}\left(p_i+1\right)^2 \\ & + \sum_{i=2}^{r-3}\left(p_i+p_{i+1}+2\right)\left(p_{i+1}+p_{i+2}+2\right) + \sum_{i=2}^{r-1}\left(p_i+1\right)\left(p_i+p_{i-1}+2\right) \\ & + \left(p_r+p_{r-1}+1\right)\left[\left(p_{r-1}+1\right)^2 + p_r^2 + p_{r-2}+1\right]. \end{aligned}$$

Proof. Let the vertices of central path P_r in Γ be labelled as $v_i, i = 1, 2, \ldots, r$. Table 6 shows edge degree partitions of the caterpillar graph. From Eq. (1.4) and Table 6, the proof is completed. □

Corollary 3.15. *Let Γ be caterpillar $T_n(p, p, \ldots, p)$ with n vertices and P_r central path graph. Then*

$$\begin{aligned} RM_2(\Gamma) = & p^3(p-1) + 2p^2(2p+1) + 2(2p+1)(p+1)(p+2) \\ & + 4(p+1)^2(p(r-3) + (r-4)) + (r-2)\frac{p(p-1)(p+1)^2}{2}. \end{aligned}$$

TABLE 6. Frequency of graph according to edge degrees of caterpillar graph

$Frequency$	$(\boldsymbol{d}(\boldsymbol{e}), \boldsymbol{d}(\boldsymbol{f})), \boldsymbol{e} \sim \boldsymbol{f}$
$p_1\left(\frac{p_1-1}{2}\right)$	(p_1, p_1)
p_1	(p_1, p_1+p_2+1)
1	(p_1+p_2+1, p_2+p_3+1)
p_2	(p_1+p_2+1, p_2+1)
p_i	$(p_i+p_{i+1}+2, p_i+1), 2 \leq i \leq r-2$
$\frac{p_i(p_i-1)}{2}$	$(p_i+1, p_i+1), 2 \leq i \leq r-1$
1	$(p_i+p_{i+1}+2, p_{i+1}+p_{i+2}+2), 2 \leq i \leq r-3$
p_i	$(p_i+p_{i-1}+2, p_i+1)\ for 3 \leq i \leq r-1$
p_{r-1}	$(p_{r-1}+1, p_r+p_{r-1}+1)$
p_r	$(p_r, p_r+p_{r-1}+1)$
$\frac{p_r(p_r-1)}{2}$	(p_r, p_r)
1	$(p_{r-1}+p_{r-2}+2, p_r+p_{r-1}+1)$

Theorem 3.16. *Let C_n^* be thorn cycle graph with $n+\sum_{i=1}^n p_i$ vertices. Then*

$$RM_1\left(C_n^*\right)=\sum_{i=1}^n p_i\left(p_i+1\right)^2++\sum_{i=1}^{n-1}\left(p_i+p_{i+1}+2\right)^2+\left(p_1+p_n+2\right)^2.$$

Proof. Let C_n^* be thorn cycle graph obtained from p_i attaching to each $v_i, i=1,2,\ldots,n$ of C_n. From the Definition 2.4, the thorn cycle graph has edge-degree partitions in Table 7. From Eq. (1.3) and Table 7, the proof is completed. □

TABLE 7. Frequency of graph according to edge degrees of the thorn cycle graph

$Frequency$	$\boldsymbol{d}(\boldsymbol{e}), \boldsymbol{e} \in \boldsymbol{E}\left(\boldsymbol{C}_{\boldsymbol{n}}^{*}\right)$
p_i	$p_i+1, for 1 \leq i \leq n$
1	$p_i+p_{i+1}+2(\bmod n), 1 \leq i \leq n$

Corollary 3.17. *Let C_n^* be thorn cycle graph obtained by attaching p thorn to each v_i vertices of C_n cycle. Then*

$$RM_1\left(C_n^*\right)=n(p+4)(p+1)^2.$$

Theorem 3.18. *Let C_n^* be thorn cycle graph obtained from p_i attaching to each v_i of C_n vertices. Then*

$$RM_2\left(C_n^*\right)=\sum_{i=1}^{n}\frac{p_i\left(p_i-1\right)\left(p_i+1\right)^2}{2}+\sum_{i=1}^{n}p_i\left(p_i+1\right)\left(2p_i+p_{i+1}+p_{i-1}+4\right)$$
$$+\sum_{i=1}^{n}\left(p_i+p_{i+1}+2\right)\left(p_{i+1}+p_{i+2}+2\right).$$

Proof. Let C_n^* be thorn cycle graph obtained from p_i attaching to each $v_i, i=1,2,\ldots,n$ of C_n. Let $n+1$ be equal to 1 and 0 be equal to n, and $n+2$ be equal to 2 for mod$n$. Then, Table 8 shows edge degree partitions of thorn cycle graph.

Table 8. Frequency of graph according to edge degree partitions of thorn cycle graph

Frequency	$(\boldsymbol{d(e)},\boldsymbol{d(f)}),\boldsymbol{e\sim f}$
$\frac{p_i(p_i-1)}{2}$	$(p_i+1,p_i+1)\,for 1\leq i\leq n$
p_i	$(p_i+1,p_i+p_{i+1}+2)\,for 1\leq i\leq n$
p_i	$(p_i+1,p_i+p_{i-1}+2)\,for 1\leq i\leq n$
1	$(p_i+p_{i+1}+2,p_{i+1}+p_{i+2}+2)\,for 1\leq i\leq n$

From Eq.(1.4) and Table 8, the proof is completed.. □

Corollary 3.19. *Let C_n^* be thorn cycle graph obtained by attaching p thorn to each v_i vertices of C_n cycle. Then*

$$RM_2\left(C_n^*\right)=\frac{n(p+1)^2\left(p^2+7p+8\right)}{2}.$$

4. THE PROPYL ETHER IMINE DENDRIMERS (PETIM)

Dendrimers are tree-like with a symmetric core and radially symmetrical molecules. These molecules have branches and exterior surfaces. It is frequently used in drug discovery and chemistry because of its chemical stability, low solubility, and cytotoxicity [1]. So, dendrimers are also studied in chemical graph theory. Kulli et al. studied Gourava indices for dendrimers [16]. Pattabiraman et al. presented the formulas for well-known indices of some dendrimers [24]. Ali et al. explored F-coindices of some dendrimers in [2]. Munir et al. investigated the M-polynomial for some dendrimers [20]. Poly (propyl ether imine) (PETIM) dendrimers are shown that non-toxic and sustained drug with respect to some dendrimers (such as Poly amido amine (PAMAM) dendrimer) [15]. Figure 4 shows structure of PETIM dendrimer with 5 branches. In this section, PETIM dendrimers, which are important in many respects, are studied. The propyl ether imine dendrimer (PETIM) graphs have $|V(PETIM[n])|=3.2^{(n+3)}-23$ and $|E(PETIM[n])|=3.2^{(n+3)}-24$ by calculate and also see [20].

Theorem 4.1. *Let $PETIM[n]$ be graph of PETIM dendrimers. Then,*

$$RM_1(PETIM[n])=52\times2^n-54.$$

Proof. Each branch of PETIM dendrimer graph have $8+2\times8+2^2\times8+\ldots+2^{(n-2)}\times8+4\times2^{(n-1)}$ edges and because of four branch, $|E(PETIM[n])|=4\times(6\times2^n-8)+8$. Each branch edge-degree are 1, 2, and 3. The number of edges which has 2 is $4\times[(8-2)+2\times(8-2)+2^2\times(8-2)+\ldots+2^{(n-2)}\times(8-2)+(4-2)\times2^{(n-1)}]+(8-2)$. The number of edges that has 3 is $4\times[1\times2+2\times2+2^2\times2+\ldots+2^{(n-2)}\times2+1\times2^{(n-1)}]+2$.

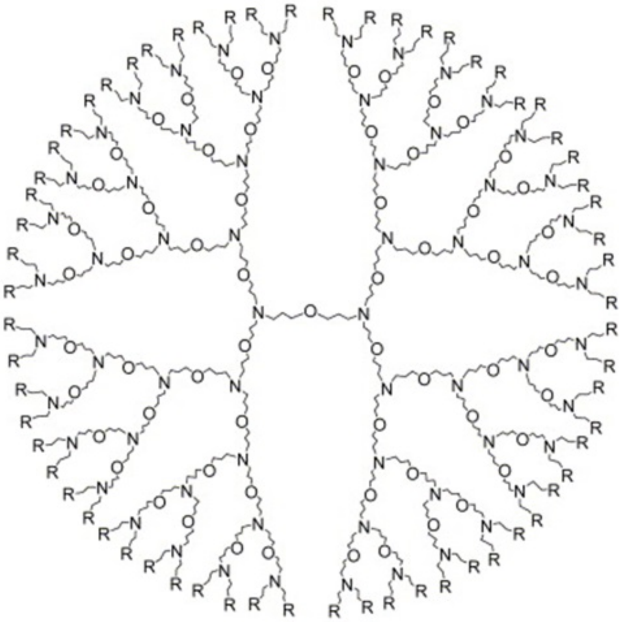

FIGURE 4. Structure of PETIM dendrimer for $n = 5$ [20].

TABLE 9. Frequency of graph according to edge degrees of the PETIM dendrimer graph.

Frequency	$\boldsymbol{d(e), e \in E\,(PETIM[n])}$
$4 \times 2^{(n-1)}$	1
$2^{(n+4)} - 18$	2
$3 \times 2^{(n+1)} - 6$	3

Then, Table 9 shows frequency of graph according to edge degrees of PETIM dendrimer graph. From Table 9 and Eq. (1.3), $52 \times 2^n - 54$ is obtained. □

Theorem 4.2. *Let $PETIM[n]$ be graph of PETIM dendrimers. Then,*

$$RM_2(PETIM[n]) = 142 \times 2^n - 150.$$

Proof. It is partitioned the edges of the molecular graph of PETIM dendrimer according to the edge degrees of neighbouring edges, the number of $d_e = 2$ and $d_f = 2$ for $e \sim f$ is $4 \times [5 + 2 \times 5 + 2^2 \times 5 + \ldots + 2^{(n-2)} \times 5 + 1 \times 2^{(n-1)}] + 5$. The number of $d_e = 2$ and $d_f = 3$ for $e \sim f$ is $4 \times [2 + 2 \times 2 + 2^2 \times 2 + \ldots + 2^{(n-2)} \times 2 + 1 \times 2^{(n-1)}] + 2$, and the number of $d_e = 3$ and $d_f = 3$ for $e \sim f$ is $4 \times [3 + 2 \times 3 + 2^2 \times 3 + \ldots + 2^{(n-2)} \times 3] + 3 \times 2$. Then, Table 10 shows the frequency of graph according to edge degrees of PETIM dendrimer graph. From Table 10 and Eq. (1.4), desired result is achieved. □

Figure 5 is graphic of the RZI of the PETIM dendrimer. This shows that as the value of n rises, that is, as the number of molecules of the PETIM dendrimer increases, the reformulated second Zagreb

TABLE 10. Frequency of graph according to edge degrees of PETIM[n]

.

$Frequency$	$(\boldsymbol{d}(\boldsymbol{e}),\boldsymbol{d}(\boldsymbol{f})),\boldsymbol{e}\sim\boldsymbol{f}$
$\frac{p_\zeta(p_\zeta-1)}{2}$	$(p_\zeta+1,p_\zeta+1)\,,\mathrm{for},1\leq\zeta\leq n$
p_ζ	$(p_\zeta+1,p_\zeta+p_{\zeta+1}+2)\,for1\leq\zeta\leq n$
p_ζ	$(p_\zeta+1,p_\zeta+p_{\zeta-1}+2)\,,for,1\leq\zeta\leq n$
1	$(p_\zeta+p_{\zeta+1}+2,p_{\zeta+1}+p_{\zeta+2}+2)\,,for,1\leq\zeta\leq n$

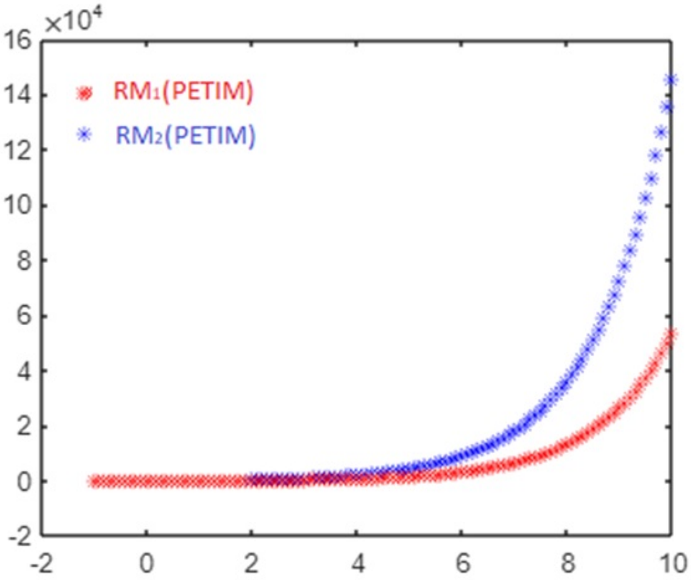

FIGURE 5. The RZI of the PETIM dendrimer.

index increases faster than the first reformulated Zagreb index. This means that the reformulated second Zagreb index value of PETIM dendrimer with the same number of molecules will be greater.

5. ALGORITHMS

In this section, the polynomial time algorithms that calculates the reformulated Zagreb indices of a Γ graph given the adjacency matrix and $|E(\Gamma)|=m$ are designed. In these algorithms, deg (v) is the degree of vertex $v\in V(\Gamma)$ and $d(e)$ is the degree of the edge $e\in E(\Gamma)$. Algorithm 1 gives the algorithm that calculates the reformulated first Zagreb index of any Γ graph. Algorithm 2 shows reformulated second Zagreb index of any Γ graph.

Algorithms 1. Compute Reformulated first Zagreb index.

```
Input: Adjacency matrix A and number of edges $|E(\Gamma)|=m$
Output: The reformulated first Zagreb index $RM_1$
$RM_1 \leftarrow 0$
$deg(v) \leftarrow 0$
```

```
$d(e) \leftarrow 0$
 for $\eta \leftarrow 1$ to $n$ do
for $\kappa \leftarrow 1$ to $n$ do
   $\deg(\eta) \leftarrow \deg(\eta) + A[\eta, \kappa]$ ;
end
end
 for $\xi \leftarrow 1$ to $m$ do
 for $\eta \leftarrow 1$ to $n-1$ do
    for $\kappa \leftarrow \eta + 1$ to n do
    If $A[\eta, \kappa] = 1$ then
   $d(\xi) \leftarrow \deg(\eta) + \deg(\kappa) - 2$ ;
    endif
    end
 end
$RM_1 \leftarrow RM_1 + d(\xi)^2$
 end
```

Algorithms 2. Compute Reformulated second Zagreb index

```
Input: Adjacency matrix A
Output: The reformulated second Zagreb index $RM_2$
$RM_2 \leftarrow 0$
$deg(v) \leftarrow 0$
for $\eta \leftarrow 1$ to $n$ do
for $\kappa \leftarrow 1$ to n do
   $\deg(\eta) \leftarrow \deg(\eta) + A[\eta, \kappa]$;
end
end
for $\eta \leftarrow 1$ to n do
for $\kappa \leftarrow 1$ to $n-1$ do
for $l \leftarrow \kappa + 1$ to n do
If $A[\eta, \kappa] = 1$ and $A[\eta, l] = 1$ then
$RM_2 \leftarrow RM_2 + (deg(\eta) + deg(\kappa) - 2)(deg(\eta) + deg(l) - 2)$;
end
end
end.
```

6. Discussions and conclusions

New drug discoveries are needed to stop and prevent these diseases, as viruses and bacteria develop resistance to drugs, diseases, and epidemics caused by new viruses increase. Therefore, in order to make these discoveries with optimum time and cost, a solution is sought with chemical graph theory in the field of mathematical chemistry. The molecular descriptors are used theoretically to predict the physical-chemical and bioactivity properties of a chemical structure.

Since tree graphs do not contain cycles, these graphs are an important field of study in theoretical graph theory, especially in computer science and many other fields. In addition, these graphs are represented the chemical structure of many drugs and molecules in the chemical graph theory. Thorny graphs are graphs obtained by adding pendent vertices to each vertex of a graph. It is also a tree graph. They represent many drugs and chemical structures in chemical graph theory, especially dendrimers.

In this study, first of all, reformulated Zagreb indices depending on the edge degree of a thorny graph of any graph and reformulated indices of special graphs such as tree graph are obtained. In the last section, Algorithms RZI for any graph are designed. In the last section, RZI of PETIM dendrimer, which is a tree graph and also a thorny tree graph, are calculated and the results are compared using the MATLAB program. As a result, the behaviour of the RM_2 index shows an asymptotically faster rate of increase than the RM_1 index. It is clear that the value of the RZI of the thorny graphs is greater than the values of the RZI of the graph. This means that for all chemical structures that have a tree graph structure such as PETIM dendrimer, the value of the indices will raise as the number of molecules in the structure raise. Moreover, the value of the second reformulated Zagreb index will grow faster than the value of the reformulated first Zagreb index. In this case, if it is desired to have large index values to predict the properties of chemicals, it is necessary to work with the reformulated second Zagreb index. The results obtained here will be useful to predict the properties of new chemicals that have or will have a tree graph structure. That is, all the results obtained will shed light on the fields of bioinformatics, mathematical chemistry, and drug design.

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