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ON THE GUTMAN INDEX OF THORN GRAPHS

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ABSTRACT. In this paper, the relation between the Gutman index of a simple connected graph and its thorn graph is stablished and several special cases of the result are examined. Results are applied to compute the Gutman index of thorn paths, thorn rods, caterpillars, thorn rings, thorn stars, Kragujevac trees, and dendrimers.

Keywords: Gutman index, degree distance, terminal Wiener index, thorn graph, dendrimer.

INTRODUCTION

Let *G* be an *n*-vertex simple connected graph with vertex set $V(G)=\{v_1,v_2,...,v_n\}$ and let $\mathrm{P}=(p_1,p_2,...,p_n)$ be an *n*-tuple of nonnegative integers. The *thorn graph* G_{P} is the graph obtained by attaching p_i pendent vertices (terminal vertices or vertices of degree one) to the vertex v_i of *G*, for $i=1,2,...,n$ (see Fig. 1).

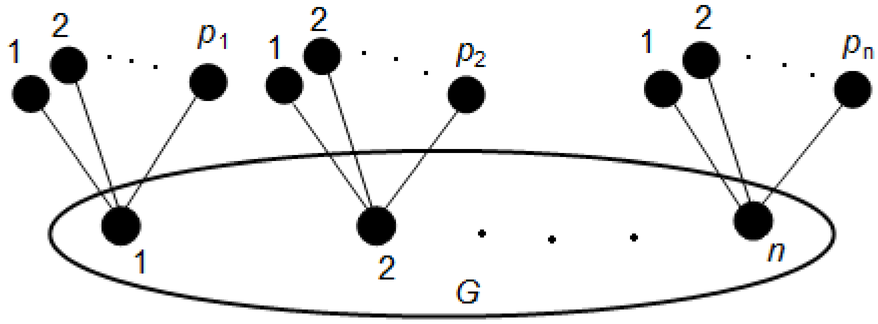
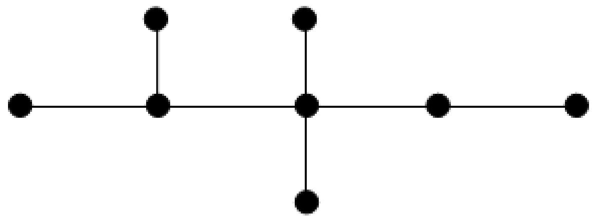


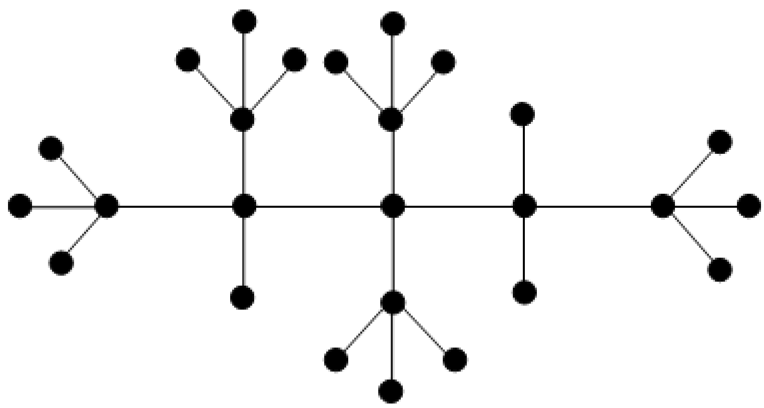
Figure 1. The thorn graph G_{P} with parameters $p_1,p_2,...,p_n$.

The p_i pendent vertices attached to the vertex v_i are called thorns of v_i. We denote the set of p_i thorns of v_i by V_i, $i=1,2,...,n$. Clearly, $V(G_{\mathrm{P}})=V(G)\cup V_1\cup V_2\cup...\cup V_n$. The concept of thorn graphs was introduced by GUTMAN (1998) and eventually found a variety of chemical applications; see (BYTAUTAS *et al.*, 2001; BONCHEV and KLEIN, 2002; VUKIČEVIĆ and

GRAOVAC, 2004; ZHOU, 2005; VUKIČEVIĆ *et al*., 2005, 2007; WALIKAR *et al*., 2006; KLEIN *et al*., 2007; HEYDARI and GUTMAN, 2010; LI, 2011; ALIZADEH *et al*., 2014; AZARI, 2014; AZARI and IRANMANESH, 2015, 2016). The motivation for the study of thorn graphs came from a particular case, namely $G_P = G_{(\gamma-\gamma_1,\gamma-\gamma_2,\ldots,\gamma-\gamma_n)}$, where γ_i is the degree of the *i*-th vertex of G and γ is a constant ($\gamma \geq \gamma_i$ for all $i = 1,2,\ldots,n$). Then the vertices of G_P are either of degree γ or of degree one. If in addition $\gamma = 4$, then the thorn graph G_P is just what CAYLEY (1874) calls a *plerogram* (a graph in which every atom is represented by a vertex and adjacent atoms are connected by a chemical bond) and POLYA (1937) a *C-H graph*. The parent graph G would then be referred to as a *kenogram* (CAYLEY, 1874) (a graph obtained from a plerogram by suppressing hydrogen atoms) or a *C-graph* (POLYA, 1937). The plerogram and kenogram of 2,3,3-trimethylpentane are depicted in Fig. 2.



(a)



(b)

Figure 2. (a) The kenogram of 2,3,3-trimethylpentane, (b) The plerogram of 2,3,3-trimethylpentane.

A *topological index* is a numeric quantity that is mathematically derived in a direct and unambiguous manner from the structural graph of a molecule. It is used in theoretical chemistry for the design of chemical compounds with given physico-chemical properties or given pharmacologic and biological activities (DIUDEA, 2001). It is well known that the study of topological indices of kenograms is much more conventional than plerograms, because of their simplicity and the fact that many topological indices give highly correlated results on plerograms and kenograms (GUTMAN *et al*., 1998). The study of thorn graphs unifies these two approaches by giving mathematical formulae that connect the values of topological indices of kenograms and plerograms.

In this paper, we study relation between the Gutman index of a simple connected graph and its thorn graph and apply the results to compute the Gutman index of thorn paths, thorn rods, caterpillars, thorn rings, thorn stars, Kragujevac trees, and dendrimers.

DEFINITIONS AND PRELIMINARIES

In this paper, we consider connected finite graphs without any loops or multiple edges. The best known and widely used topological index is the *Wiener index* introduced by WIENER (1947), who used it for modeling the shape of organic molecules and for calculating several of their physico-chemical properties. The Wiener index of a graph G is defined as the sum of distances between all pairs of vertices of G,

$$W(G)=\sum_{\{u,v\}\subseteq V(G)} d_G(u,v),$$

where $d_G(u,v)$ denotes the distance between the vertices u and v in G.

The *degree distance* was introduced by DOBRYNIN and KOCHETOVA (1994) and at the same time by GUTMAN (1994) as a weighted version of the Wiener index. The degree distance of a graph G is defined as

$$DD(G)=\sum_{\{u,v\}\subseteq V(G)} [d_G(u)+d_G(v)]d_G(u,v).$$

In fact, if T is a tree on n vertices, the Wiener index and degree distance are closely related by $DD(T)=4W(T)-n(n-1)$; see (GUTMAN, 1994).

The *Gutman index* (also known as *Schultz index of the second kind*) was introduced by GUTMAN (1994) as a kind of vertex-valency-weighted sum of the distances between all pairs of vertices in a graph. Gutman revealed that in the case of acyclic structures, the index is closely related to the Wiener index and reflects precisely the same structural features of a molecular as the Wiener index does. The Gutman index of a graph G is defined as

$$Gut(G)=\sum_{\{u,v\}\subseteq V(G)} d_G(u)d_G(v)d_G(u,v).$$

We refer the reader to (FENG and LIU, 2011; ANDOVA *et al.*, 2012; CHEN, 2016; KNOR *et al.*, 2014; GUTMAN, 2016; AZARI, 2016; AZARI and DIVANPOUR, 2017) for more information on the Gutman index and degree distance.

The concept of *terminal Wiener index* was put forward by GUTMAN *et al*. (2009). Somewhat later, but independently, SZÉKELY *et al*. (2011) arrived at the same idea. The terminal Wiener index $TW(G)$ of a graph G is defined as the sum of distances between all pairs of its pendent vertices,

$$TW(G)=\sum_{\{u,v\}\subseteq V'(G)} d_G(u,v).$$

where $V'(G)$ is the set of all pendent vertices of G.

For $u\in V(G)$, we define the quantity $TW_G(u)$ as the sum of distances between u and all pendent vertices of G,

$$TW_G(u)=\sum_{v\in V'(G)} d_G(u,v).$$

It is easy to see that, $TW(G)=\frac{1}{2}\sum_{u\in V'(G)} TW_G(u)$.

RESULTS AND DISCUSSION

In this section, we establish relation between the Gutman index of a simple connected graph G and its thorn graph G_{P}, and examine several special cases of the result.

Theorem 1. Let G be a connected n-vertex graph with vertex set $V(G)=\{v_1, v_2, ..., v_n\}$, and let G_{P} be the thorn graph of G with nonnegative parameters $p_1, p_2, ..., p_n$. Then

$$Gut(G_{\mathrm{P}}) = Gut(G) + 2\sum_{1\le i<j\le n}(p_j d_G(v_i) + p_i d_G(v_j))d_G(v_i,v_j) + 4\sum_{1\le i<j\le n} p_i p_j d_G(v_i,v_j) \qquad (1)$$

$$+2(\sum_{i=1}^{n} p_i)^2 + (2|E(G)|-1)\sum_{i=1}^{n} p_i \ .$$

Proof. By definition of the Gutman index, we have

$$Gut(G_{\mathrm{P}}) = \sum_{\{u,v\}\subseteq V(G_{\mathrm{P}})} d_{G_{\mathrm{P}}}(u) d_{G_{\mathrm{P}}}(v) d_{G_{\mathrm{P}}}(u,v) .$$

By definition of the graph G_{P}, the above sum can be partitioned into four sums as follows.

The first sum S_1 consists of contriutions to $Gut(G_{\mathrm{P}})$ of pairs of vertices from G,

$$S_1 = \sum_{1\le i<j\le n} d_{G_{\mathrm{P}}}(v_i) d_{G_{\mathrm{P}}}(v_j) d_{G_{\mathrm{P}}}(v_i,v_j)$$

$$= \sum_{1\le i<j\le n}(d_G(v_i)+p_i)(d_G(v_j)+p_j) d_G(v_i,v_j)$$

$$= Gut(G) + \sum_{1\le i<j\le n}(p_j d_G(v_i) + p_i d_G(v_j))d_G(v_i,v_j) + \sum_{1\le i<j\le n} p_i p_j d_G(v_i,v_j) .$$

The second sum S_2 consists of contriutions to $Gut(G_{\mathrm{P}})$ of pairs of vertices from V_i for all $1 \le i \le n$,

$$S_2 = \sum_{i=1}^{n} \sum_{\{u,v\}\subseteq V_i} d_{G_{\mathrm{P}}}(u) d_{G_{\mathrm{P}}}(v) d_{G_{\mathrm{P}}}(u,v) = \sum_{i=1}^{n} \sum_{\{u,v\}\subseteq V_i} 1\times 1\times 2 = 2\sum_{i=1}^{n}\binom{p_i}{2} = \sum_{i=1}^{n} p_i{}^2 - \sum_{i=1}^{n} p_i \ .$$

The third sum S_3 is taken over all pairs of vertices such that one of them, u, is in G, and the other one, v, is in V_j for $1 \le j \le n$. So

$$S_3 = \sum_{i=1}^{n}\sum_{j=1}^{n}\sum_{u=v_i}\sum_{v\in V_j} d_{G_{\mathrm{P}}}(u) d_{G_{\mathrm{P}}}(v) d_{G_{\mathrm{P}}}(u,v)$$

$$= \sum_{i=1}^{n}\sum_{j=1}^{n}\sum_{u=v_i}\sum_{v\in V_j}(d_G(v_i)+p_i)\times 1\times(d_G(v_i,v_j)+1)$$

$$= \sum_{i=1}^{n} d_G(v_i)\sum_{j=1}^{n} p_j d_G(v_i,v_j) + \sum_{i=1}^{n} d_G(v_i)\sum_{j=1}^{n} p_j + \sum_{i=1}^{n} p_i \sum_{j=1}^{n} p_j d_G(v_i,v_j) + \sum_{i=1}^{n} p_i \sum_{j=1}^{n} p_j \ .$$

It is easy to check that

$$\sum_{i=1}^{n} d_G(v_i)\sum_{j=1}^{n} p_j d_G(v_i,v_j) = \sum_{1\le i<j\le n}(p_j d_G(v_i) + p_i d_G(v_j))d_G(v_i,v_j) .$$

Hence

$$S_3 = \sum_{1\le i<j\le n}(p_j d_G(v_i) + p_i d_G(v_j))d_G(v_i,v_j) + 2\sum_{1\le i<j\le n} p_i p_j d_G(v_i,v_j) + (\sum_{i=1}^{n} p_i)^2 + 2|E(G)|\sum_{i=1}^{n} p_i \ . \qquad (2)$$

The fourth sum S_4 is taken over all pairs of vertices such that one of them, *u*, is in V_i, and the other one, *v*, is in V_j, where $1 \le i \ne j \le n$. So

$$S_4 = \sum_{1\le i<j\le n}\sum_{u\in V_i}\sum_{v\in V_j} d_{G_P}(u)d_{G_P}(v)d_{G_P}(u,v) = \sum_{1\le i<j\le n}\sum_{u\in V_i}\sum_{v\in V_j} 1\times 1\times (d_G(v_i,v_j)+2)$$
$$= \sum_{1\le i<j\le n} p_i p_j d_G(v_i,v_j) + 2\sum_{1\le i<j\le n} p_i p_j \ .$$

It is easy to check that

$$2\sum_{1\le i<j\le n} p_i p_j = \sum_{i=1}^{n}\sum_{j=1}^{n} p_i p_j - \sum_{i=1}^{n} p_i^{\,2} = (\sum_{i=1}^{n} p_i)^2 - \sum_{i=1}^{n} p_i^{\,2} \ .$$

Hence

$$S_4 = \sum_{1\le i<j\le n} p_i p_j d_G(v_i,v_j) + (\sum_{i=1}^{n} p_i)^2 - \sum_{i=1}^{n} p_i^{\,2} \ .$$

Eq. (1) is obtained by adding S_1, S_2, S_3, S_4, and simplifying the resulting expression.

For every connected graph *G*, we define

$$\Psi(G) = \sum_{u\in V(G)-V'(G)} d_G(u) TW_G(u) \ .$$

In the following theorem, we find a formula for $\Psi(G_P)$.

Theorem 2. Let *G* be a connected n-vertex graph with vertex set $V(G) = \{v_1, v_2, ..., v_n\}$, and let G_P be the thorn graph of *G* with parameters $p_1, p_2, ..., p_n$ such that for every pendent vertex v_i of *G*, $p_i > 0$. Then

$$\Psi(G_P) = \sum_{1\le i<j\le n}(p_j d_G(v_i) + p_i d_G(v_j))d_G(v_i,v_j) + 2\sum_{1\le i<j\le n} p_i p_j d_G(v_i,v_j) + (\sum_{i=1}^{n} p_i)^2 + 2|E(G)|\sum_{i=1}^{n} p_i \ . \quad (3)$$

Proof. Since for every pendent vertex v_i of *G*, $p_i > 0$, so $V'(G_P) = V_1 \cup V_2 \cup ... \cup V_n$ and $V(G_P) - V'(G_P) = V(G)$. Then

$$\Psi(G_P) = \sum_{u\in V(G)} d_{G_P}(u) TW_{G_P}(u) = \sum_{u\in V(G)}\sum_{v\in V'(G_P)} d_{G_P}(u)d_{G_P}(v)d_{G_P}(u,v) \ .$$

One can easily see that, $\Psi(G_P)$ is the contribiutions to $Gut(G_P)$ of all pairs of vertices $\{u,v\}$ of G_P such that one of them, *u*, is in *G*, and the other one, *v*, is in V_j for $1 \le j \le n$. So $\Psi(G_P)$ is equal to the sum S_3 in the proof of Theorem 1. Now using Eq. (2), we can get Eq. (3).

As a direct consequence of Theorem 2, we get the following corollary which will be used in the next section.

Corollary 1. Let *G* be a connected *n*-vertex graph with *k* pendent vertices, and let G_P be the thorn graph of *G* obtained by attaching $p > 0$ pendent vertices to each pendent vertex of *G*. Then

$$\Psi(G_P) = 2p(p+1)TW(G) + p\Psi(G) + kp(kp + 2|E(G)|) \ . \qquad (4)$$

Proof. Let $V(G)=\{v_1,v_2,...,v_n\}$, and without loss of generality let $V'(G)=\{v_1,v_2,...,v_k\}$. By setting $p_1=p_2=...=p_k=p$ and $p_{k+1}=p_{k+2}=...=p_n=0$ in Eq. (3), we obtain

$$\Psi(G_P)=\sum_{1\le i<j\le k}(p\times 1+p\times 1)d_G(v_i,v_j)+\sum_{k+1\le i<j\le n}[0\times d_G(v_i)+0\times d_G(v_j)]d_G(v_i,v_j)$$

$$+\sum_{i=1}^{k}\sum_{j=k+1}^{n}[0\times d_G(v_i)+p\times d_G(v_j)]d_G(v_i,v_j)+2\sum_{1\le i<j\le k}p^2 d_G(v_i,v_j)$$

$$+2\sum_{k+1\le i<j\le n}0^2 d_G(v_i,v_j)+2\sum_{i=1}^{k}\sum_{j=k+1}^{n}p\times 0\times d_G(v_i,v_j)+(kp)^2+2kp|E(G)|.$$

Using the relations $\sum_{1\le i<j\le k}d_G(v_i,v_j)=TW(G)$ and $\sum_{i=1}^{k}\sum_{j=k+1}^{n}d_G(v_j)d_G(v_i,v_j)=\Psi(G)$, we get Eq. (4).

Now, we express some special cases of Theorem 1.

Corollary 2. Let G be a connected n-vertex graph, and let G_P be the thorn graph of G with parameters $p_1=p_2=...=p_n=p$, where p is a nonnegative integer. Then

$$Gut(G_P)=Gut(G)+2pDD(G)+4p^2W(G)+np(2np+2|E(G)|-1). \qquad (5)$$

Corollary 3. Let G be a connected n-vertex graph with k pendent vertices, and let G_P be the thorn graph of G obtained by attaching $p\ge 0$ pendent vertices to each pendent vertex of G. Then

$$Gut(G_P)=Gut(G)+4p(p+1)TW(G)+2p\Psi(G)+kp(2kp+2|E(G)|-1). \qquad (6)$$

Proof. Let $V(G)=\{v_1,v_2,...,v_n\}$, and without loss of generality let $V'(G)=\{v_1,v_2,...,v_k\}$. By setting $p_1=p_2=...=p_k=p$ and $p_{k+1}=p_{k+2}=...=p_n=0$ in Eq. (1), we can get Eq. (6).

Corollary 4. Let G be a connected n-vertex graph with vertex set $V(G)=\{v_1,v_2,...,v_n\}$, and let G_P be the thorn graph of G with parameters $p_1,p_2,...,p_n$, where $p_i=d_G(v_i)$, $i=1,2,...,n$. Then

$$Gut(G_P)=9Gut(G)+12|E(G)|^2-2|E(G)|.$$

Corollary 5. Let G be a connected n-vertex graph with vertex set $V(G)=\{v_1,v_2,...,v_n\}$, and let γ be an integer with the property $\gamma\ge d_G(v_i)$, for $i=1,2,...,n$. Let G_P be the thorn graph of G with parameters $p_1,p_2,...,p_n$, where $p_i=\gamma-d_G(v_i)$, $i=1,2,...,n$. Then

$$Gut(G_P)=Gut(G)+4\gamma^2W(G)-2\gamma DD(G)+(n\gamma-2|E(G)|)(2n\gamma-2|E(G)|-1).$$

Proof. It is easy to see that

$$\sum_{i=1}^{n}p_i=n\gamma-2|E(G)|,\quad \sum_{1\le i<j\le n}(p_j d_G(v_i)+p_i d_G(v_j))d_G(v_i,v_j)=\gamma DD(G)-2Gut(G),$$

$$\sum_{1\le i<j\le n}p_i p_j d(v_i,v_j|G)=\gamma^2W(G)-\gamma DD(G)+Gut(G).$$

Now using Eq. (1), we can get the desired result.

APPLICATIONS

In this section, we apply the results of the previous section to compute the Gutman index of various classes of chemical graphs and nanostructures derived from thorn graphs. Let P_n, S_n, and C_n denote the n-vertex path, star and cycle, respectively. It is easy to see that

$$Gut(P_n)=\frac{(n-1)(2n^2-4n+3)}{3},\ Gut(S_n)=(n-1)(2n-3),\ Gut(C_n)=\begin{cases}\frac{n(n^2-1)}{2} & if\ n\ is\ odd,\\ \frac{n^3}{2} & if\ n\ is\ even.\end{cases}$$

Thorn paths

The *thorn path* $P_{n,p,k}$ is obtained from the path P_n by adding p neighbors to each of its nonterminal vertices and k neighbors to each of its terminal vertices (see Fig. 3). Consider the path P_n and choose a labeling for its vertices such that its two terminal vertices have numbers 1 and n and its nonterminal vertices have numbers $2,3,\ldots,n-1$ as shown in Fig. 3. Then, $P_{n,p,k}$ can be considered as the thorn graph $(P_n)_P$, where P is the n-tuple $\mathrm{P}=(k,p,\ldots,p,k)$. Using Eq. (1), we get the following theorem.

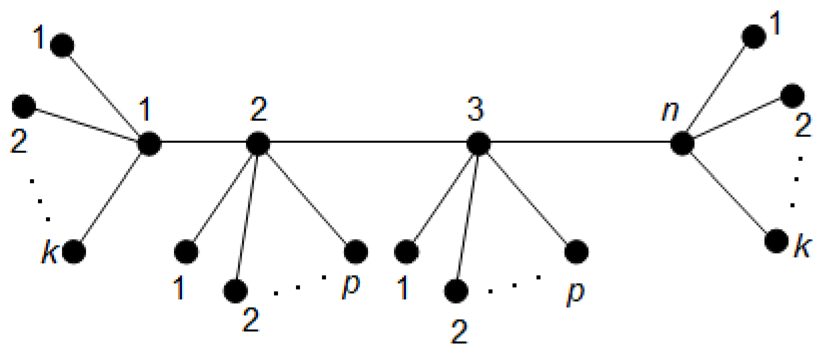


Figure 3. The thorn path $P_{n,p,k}$.

Theorem 3. Let $n\geq 2$ and let p and k be any nonnegative integers. Then

$$Gut(P_{n,p,k})=\frac{(n-1)(2n^2-4n+3)}{3}+\frac{2p^2}{3}(n^3-3n^2-n+6)+\frac{p}{3}(4n^3-12n^2+5n+6) \qquad (7)$$
$$+4k^2(n+1)+2k(2n^2-2n-1)+4kp(n-2)(n+1).$$

Thorn rods

The *thorn rod* $P_{n,m}$ is a graph which includes a linear chain (termed "rod") of n vertices and degree-m terminal vertices at each of the two rod ends, where $m\geq 2$ (see Fig. 4). It is easy to see that $P_{n,m}\cong P_{n,0,m-1}$. Using Eq. (7), we get the following corollary.

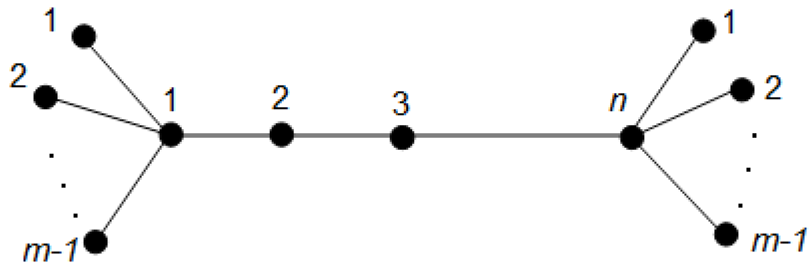


Figure 4. The thorn rod $P_{n,m}$.

Corollary 6. Let $n,m \ge 2$. Then

$$Gut(P_{n,m}) = \frac{(n-1)(2n^2-4n+3)}{3} + 4(m-1)^2(n+1) + 2(m-1)(2n^2-2n-1).$$

Caterpillars

The *caterpillar* $T^*(m,n)$ is a thorn graph whose parent graph is the path P_n and whose n nonterminal vertices are of the same degree $m > 2$ (see Fig. 5). It is easy to see that $T^*(m,n) \cong P_{n,m-2,m-1}$. Using Eq. (7), we get the following corollary.

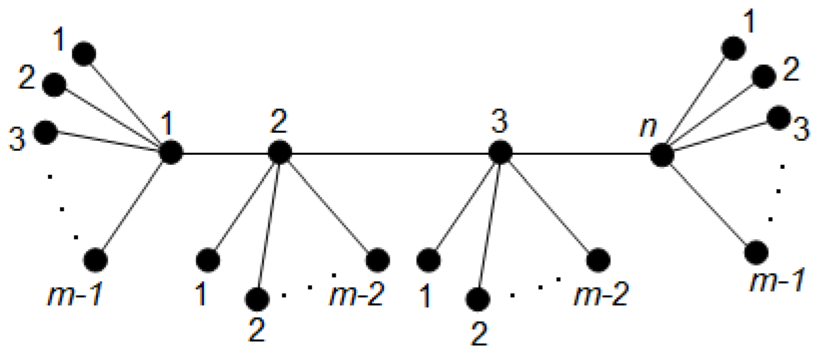


Figure 5. The caterpillar $T^*(m,n)$.

Corollary 7. Let $n \ge 2$ and $m > 2$. Then

$$Gut(T^*(m,n)) = \frac{(n-1)(2n^2-4n+3)}{3} + \frac{2(m-2)^2}{3}(n^3-3n^2-n+6) + \frac{m-2}{3}(4n^3-12n^2+5n+6)$$
$$+ 4(m-1)^2(n+1) + 2(m-1)(2n^2-2n-1) + 4(m-1)(m-2)(n-2)(n+1).$$

Thorn rings

The *m-thorn ring* $C_{n,m}$ has a cycle C_n as the parent, and $m-2$ thorns at each cycle vertex, where $m > 2$. The 3-thorn ring $C_{6,3}$ is depicted in Fig. 6. The *m*-thorn ring $C_{n,m}$ can be considered as the thorn graph $(C_n)_P$, where P is the *n*-tuple $\mathrm{P} = (m-2, m-2, ..., m-2)$. Using Eq. (5) and the fact that $Gut(C_n) = DD(C_n) = 4W(C_n)$, we get the following theorem.

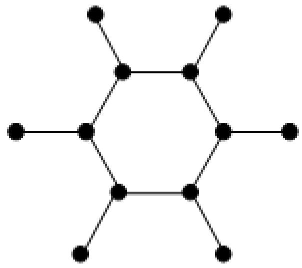


Figure 6. The 3-thorn ring $C_{6,3}$.

Theorem 4. Let $n, m \geq 3$. Then

$$Gut(C_{n,m}) = \begin{cases} \dfrac{n(n^2-1)}{2}(m-1)^2 + n(m-2)(2n(m-1)-1) & n \text{ is odd}, \\ \dfrac{n^3}{3}(m-1)^2 + n(m-2)(2n(m-1)-1) & n \text{ is even}. \end{cases}$$

Thorn stars

The *thorn star* $S_{n,p,k}$ is obtained from the star S_n by adding *p* neighbors to the center of the star and *k* neighbors to its terminal vertices (see Fig. 7). Consider the star S_n and choose a labeling for its vertices such that its terminal vertices have numbers $1,2,\dots,n-1$ and its central vertex has number *n* as shown in Fig. 7. Then, $S_{n,p,k}$ can be considered as the thorn graph $(S_n)_P$, where P is the *n*-tuple $\mathrm{P} = (k, k, \dots, k, p)$. Using Eq. (1), we get the following theorem.

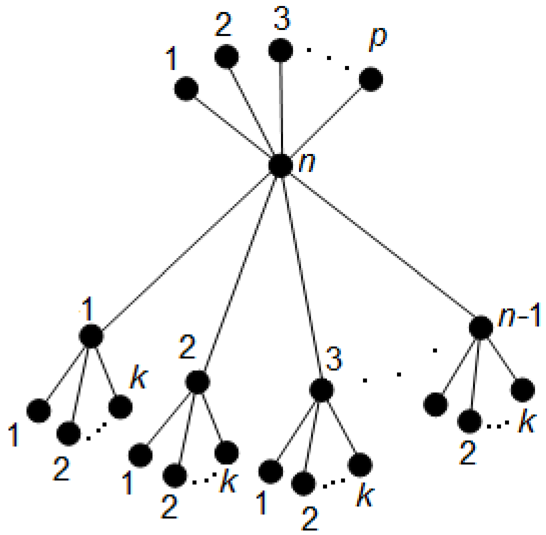


Figure 7. The thorn star $S_{n,p,k}$.

Theorem 5. Let $n \geq 3$ and let *p* and *k* be any nonnegative integers. Then

$$Gut(S_{n,p,k}) = (n-1)(2n-3) + k(8n^2 - 21n + 13) + 2k^2(3n^2 - 8n + 5) \tag{8}$$

$$+8pk(n-1)+p(4n-5)+2p^2 .$$

By setting $p=0$ in Eq. (8), we get the following corollary.

Corollary 8. Let $n \geq 3$ and let k be any nonnegative integer. Then

$$Gut(S_{n,0,k}) = (n-1)(2n-3) + k(8n^2 - 21n + 13) + 2k^2(3n^2 - 8n + 5) .$$

Consider the star graph S_n and choose a labeling for its vertices such that its terminal vertices have numbers $1,2,...,n-1$ and its central vertex has number n. Let $S_n(p_1, p_2,..., p_{n-1})$ denote the thorn star obtained by attaching p_i terminal vertices to the vertex i of S_n for $i=1,2,...,n-1$ (see Fig. 8). Using Eq. (1), we get the following theorem.

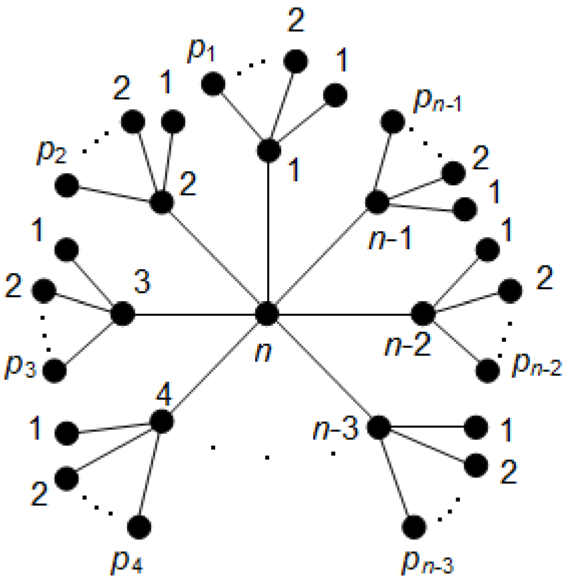


Figure 8. The thorn star $S_n(p_1, p_2,..., p_{n-1})$.

Theorem 6. Let $n \geq 3$ and let $p_1, p_2,..., p_{n-1}$ be nonnegative integers. Then

$$Gut(S_n(p_1, p_2,..., p_{n-1})) = (n-1)(2n-3) + 6(\sum_{i=1}^{n-1} p_i)^2 - 4\sum_{i=1}^{n-1} p_i^{\,2} + (8n-13)\sum_{i=1}^{n-1} p_i . \quad (9)$$

Kragujevac trees

Let P_3 be the 3-vertex path rooted at one of its terminal vertices. For $k = 2,3,...$, construct the rooted tree B_k by identifying the roots of k copies of P_3. The vertex obtained by identifying the roots of P_3-trees is the root of B_k. Examples illustrating the structure of the rooted tree B_k are depicted in Fig. 9.

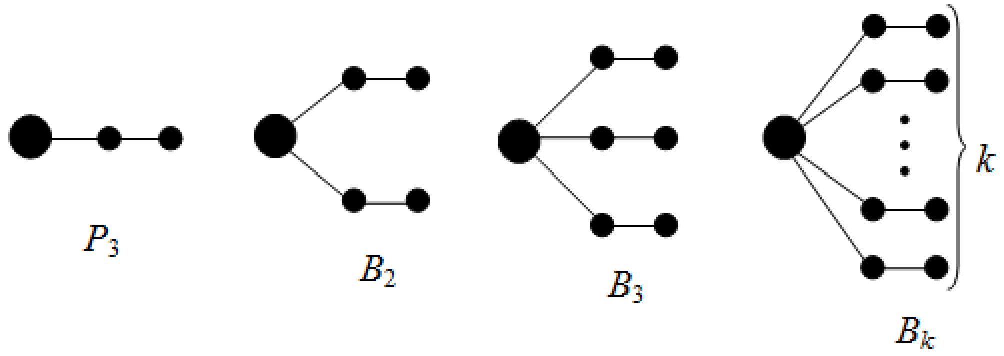


Figure 9. The rooted trees B_2, B_3, and B_k. Their roots are indicated by large dots.

According to GUTMAN (2014), a *Kragujevac tree T* is a tree possessing a vertex of degree $d \geq 2$, adjacent to the roots of $B_{p_1}, B_{p_2}, ..., B_{p_d}$, where $p_1, p_2, ..., p_d \geq 2$. This vertex is said to be the central vertex of *T*, whereas d is the degree of *T*. The subgraphs $B_{p_1}, B_{p_2}, ..., B_{p_d}$ are the branches of *T*. Recall that some (or all) branches of *T* may be mutually isomorphic. We denote the Kragujevac tree of degree d with branches $B_{p_1}, B_{p_2}, ..., B_{p_d}$ by $Kg(p_1, p_2, ..., p_d)$. A typical Kragujevac tree is depicted in Fig. 10.

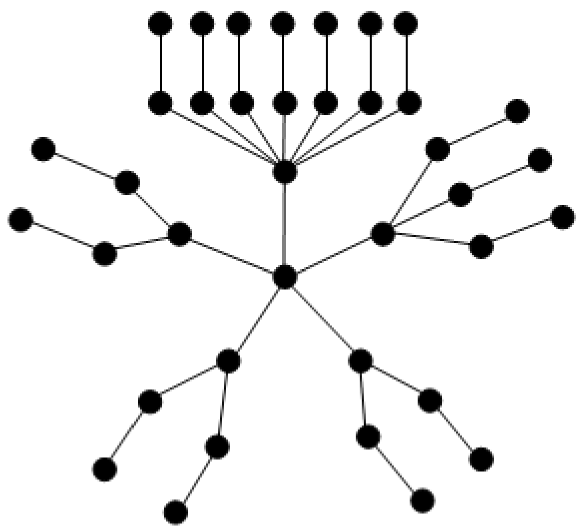


Figure 10. The Kragujevac tree $Kg(7,3,2,2,2)$.

Theorem 7. The Gutman index of the Kragujevac tree $Kg(p_1, p_2, ..., p_d)$ is given by

$$Gut(Kg(p_1, p_2, ..., p_d)) = d(2d-1) + 32(\sum_{i=1}^{d} p_i)^2 - 16\sum_{i=1}^{d} p_i^{\,2} + (20d-18)\sum_{i=1}^{d} p_i \,. \qquad (10)$$

Proof. The Kragujevac tree $Kg(p_1, p_2, ..., p_d)$ can be considered as the thorn graph obtained from the thorn star $S_{d+1}(p_1, p_2, ..., p_d)$ by attaching a pendent vertex to its pendent vertices. By setting $G = S_{d+1}(p_1, p_2, ..., p_d)$, $p = 1$, $k = \sum_{i=1}^{d} p_i$, and $|E(G)| = \sum_{i=1}^{d} p_i + d$ in Eq. (6), we obtain

$$Gut(Kg(p_1, p_2, ..., p_d)) = Gut(S_{d+1}(p_1, p_2, ..., p_d)) + 8TW(S_{d+1}(p_1, p_2, ..., p_d)) \qquad (11)$$

$$+2\Psi(S_{d+1}(p_1, p_2,..., p_d)) + (\sum_{i=1}^{d} p_i)(4\sum_{i=1}^{d} p_i + 2d - 1) .$$

By Eq. (9), we have

$$Gut(S_{d+1}(p_1, p_2,..., p_d)) = d(2d-1) + 6(\sum_{i=1}^{d} p_i)^2 - 4\sum_{i=1}^{d} p_i^{\,2} + (8d-5)\sum_{i=1}^{d} p_i \; .$$

One can easily check that,

$$\begin{aligned} TW(S_{d+1}(p_1, p_2,..., p_d)) &= \sum_{i=1}^{d} 2\binom{p_i}{2} + \sum_{1\le i<j\le d} 4 p_i p_j = \sum_{i=1}^{d} p_i^{\,2} - \sum_{i=1}^{d} p_i + 2[(\sum_{i=1}^{d} p_i)^2 - \sum_{i=1}^{d} p_i^{\,2}] \\ &= 2(\sum_{i=1}^{d} p_i)^2 - \sum_{i=1}^{d} p_i^{\,2} - \sum_{i=1}^{d} p_i \; , \end{aligned}$$

$$\begin{aligned} \Psi(S_{d+1}(p_1, p_2,..., p_d)) &= \sum_{i=1}^{d} (p_i + 1)[p_i \times 1 + 3(\sum_{j=1}^{d} p_j - p_i)] + 2d\sum_{i=1}^{d} p_i \\ &= \sum_{i=1}^{d} (3p_i \sum_{j=1}^{d} p_j - 2p_i^{\,2} + 3\sum_{j=1}^{d} p_j - 2p_i) + 2d\sum_{i=1}^{d} p_i \\ &= 3(\sum_{i=1}^{d} p_i)^2 - 2\sum_{i=1}^{d} p_i^{\,2} + (5d-2)\sum_{i=1}^{d} p_i \; . \end{aligned}$$

Substituing the above formulae in Eq. (11), we can get Eq. (10).

Dendrimers

Let D_0 be the graph depicted in Fig. 11.

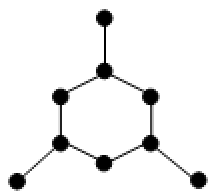


Figure 11. The dendrimer graph D_0.

For positive integers p and h, let $D_{p,h}$ be a series of dendrimers obtained by attaching p pendent vertices to each pendent vertex of $D_{p,h-1}$ and let $D_{p,0} = D_0$. We can also introduce the $D_{p,h}$ as the thorn graph obtained by attaching p pendent vertices to each pendent vertex of $D_{p,h-1}$. This molecular structure can be encountered in real chemistry, e.g. in some tertiary phosphine dendrimers. Some examples of this kind of dendrimers are shown in Fig. 12.

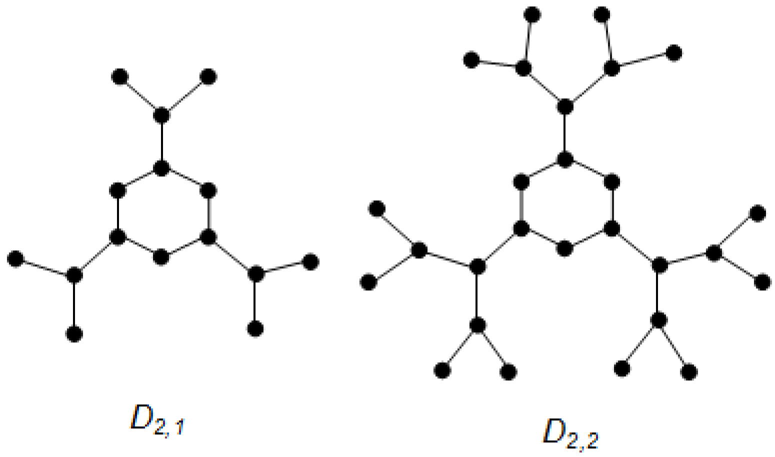


Figure 12. The dendrimer graphs $D_{p,h}$, for p=2 and h=1,2.

For a fixed positive integer p, let k_h denote the number of pendent vertices of $D_{p,h}$, $h \geq 0$. Obviously, $k_h = pk_{h-1}$ and $|E(D_{p,h})| = |E(D_{p,h-1})| + 3p^h$. So for every $h \geq 0$, we have

$$k_h = 3p^h, \ |E(D_{p,h})| = 6 + 3\sum_{i=0}^{h} p^i.$$

It is easy to check that $TW(D_0) = 12$. In (Azari and Iranmanesh, 2016), an explicit formula for computing the terminal Wiener index of the dendrimer graph $D_{p,h}$ was computed.

Theorem 8. (Azari and Iranmanesh, 2016) Let p and h be positive integers. The terminal Wiener index of the dendrimer graph $D_{p,h}$ is given by

$$TW(D_{p,h}) = (9h+12)p^{2h} - 3p^h \sum_{i=0}^{h-1} p^i . \qquad (12)$$

It is easy to check that $\Psi(D_0) = 111$ and $Gut(D_0) = 291$. In the following theorem, we present recurrence relations for computing $\Psi(D_{p,h})$ and $Gut(D_{p,h})$. Results are deduced from Eqs. (4) and (6), and the proof of the theorem is therefore omitted.

Theorem 9. Let p and h be positive integers. Then

$$\Psi(D_{p,h}) = 2p(p+1)TW(D_{p,h-1}) + p\Psi(D_{p,h-1}) + 3p^h(3p^h + 12 + 6\sum_{i=0}^{h-1} p^i), \qquad (13)$$

$$Gut(D_{p,h}) = Gut(D_{p,h-1}) + 4p(p+1)TW(D_{p,h-1}) + 2p\Psi(D_{p,h-1}) + 3p^h(11 + 6\sum_{i=0}^{h} p^i). \qquad (14)$$

Using Eqs. (12)-(14), we can compute the Gutman index of the dendrimer graph $D_{p,h}$ for every positive integers p and h.

For example, by setting $h = 1$ in Eqs. (12)-(14), we get

$TW(D_{p,1}) = 21p^2 - 3p$,

$\Psi(D_{p,1}) = 2p(p+1)TW(D_0) + p\Psi(D_0) + 3p(3p + 12 + 6) = 33p^2 + 189p$,

$$Gut(D_{p,1}) = Gut(D_0) + 4p(p+1)TW(D_0) + 2p\Psi(D_0) + 3p[11+6(1+p)] = 66p^2 + 321p + 291 .$$

By setting $h=2$ in Eqs. (12)-(14), we get

$$TW(D_{p,2}) = 30p^4 - 3p^3 - 3p^2 ,$$

$$\Psi(D_{p,2}) = 2p(p+1)TW(D_{p,1}) + p\Psi(D_{p,1}) + 3p^2[3p^2 + 12 + 6(1+p)] = 51p^4 + 87p^3 + 237p^2 ,$$

$$Gut(D_{p,2}) = Gut(D_{p,1}) + 4p(p+1)TW(D_{p,1}) + 2p\Psi(D_{p,1}) + 3p^2[11+6(1+p+p^2)]$$
$$= 102p^4 + 156p^3 + 483p^2 + 321p + 291 .$$

By setting $h=3$ in Eqs. (12)-(14), we get

$$TW(D_{p,3}) = 39p^6 - 3p^5 - 3p^4 - 3p^3 ,$$

$$\Psi(D_{p,3}) = 2p(p+1)TW(D_{p,2}) + p\Psi(D_{p,2}) + 3p^3[3p^3 + 12 + 6(1+p+p^2)]$$
$$= 69p^6 + 123p^5 + 93p^4 + 285p^3 ,$$

$$Gut(D_{p,3}) = Gut(D_{p,2}) + 4p(p+1)TW(D_{p,2}) + 2p\Psi(D_{p,2}) + 3p^3[11+6(1+p+p^2+p^3)]$$
$$= 138p^6 + 228p^5 + 270p^4 + 669p^3 + 483p^2 + 321p + 291 .$$

By setting $h=4$ in Eqs. (12)-(14), we get

$$TW(D_{p,4}) = 48p^8 - 3p^7 - 3p^6 - 3p^5 - 3p^4 ,$$

$$\Psi(D_{p,4}) = 2p(p+1)TW(D_{p,3}) + p\Psi(D_{p,3}) + 3p^4[3p^4 + 12 + 6(1+p+p^2+p^3)]$$
$$= 87p^8 + 159p^7 + 129p^6 + 99p^5 + 333p^4 ,$$

$$Gut(D_{p,4}) = Gut(D_{p,3}) + 4p(p+1)TW(D_{p,3}) + 2p\Psi(D_{p,3}) + 3p^4[11+6(1+p+p^2+p^3+p^4)]$$
$$= 174p^8 + 300p^7 + 378p^6 + 408p^5 + 879p^4 + 669p^3 + 483p^2 + 321p + 291 .$$

The Gutman index of $D_{p,h}$ for $p=2,3$ and $h \le 4$ is computed in Tab. 1.

Table 1. The Gutman index of the dendrimer graphs $D_{p,h}$ for $p=2,3$ and $h \le 4$.

h	Gut($D_{2,h}$)	Gut($D_{3,h}$)
0	291	291
1	1197	1848
2	5745	18075
3	28665	201540
4	142473	2267283

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