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Laplacian coefficients of trees

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LAPLACIAN COEFFICIENTS OF TREES

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Abstract. Let G be a simple and undirected graph with Laplacian polynomial $\psi(G,\lambda) = \sum_{k=0}^{n}(-1)^{n-k}c_k(G)\lambda^k$. In this paper, exact formulas for the coefficient c_{n-4} and the number of $4-$matchings with respect to the Zagreb indices of a given tree are presented. The chemical trees with first through the fifteenth greatest $c_{n-4}-$values are also determined.

1. Introduction

A *graph* G consists of two sets $V = V(G)$ and $E = E(G)$. The elements of V are called the *vertices* of G and the elements of E are *edges* of this graph. Each edge is a $2-$element subset of vertices $\{x, y\}$ which is denoted by xy. A *chemical graph* is a graph in which $\Delta(G) \leq 4$, where $\Delta(G)$ is the maximum degree of vertices in G and a *tree* is a connected graph without cycles. The vertex degree of $v \in V(G)$, $deg_G(v)$, is defined as the number of edges incident to v and $N_G(v)$ denotes the set of all vertices adjacent to v. The distance between two vertices $x, y \in V(G)$, $d(x, y)$, is defined as the number of edges in a shortest path connecting them. The summation of all such numbers is called the Wiener index of G denoted by $W(G)$.

For subset E of $E(G)$, we denote the subgraph of G obtained by deleting the edges of E by $G - E$. If $E = \{uv\}$, the subgraphs $G - E$ will be written as $G - uv$ for short. In addition, for any two nonadjacent vertices x and y of graph G, let $G + xy$ be the graph obtained from G by adding an xy edge. If two vertices x and y are adjacent then we write $x \sim y$. The *path* and *star* on $n-$vertices are denoted by P_n and S_n, respectively. The set of all $n-$vertex chemical trees is denoted by $\mathcal{CT}(n)$.

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Suppose $\mathcal{G}$ denotes the set of all graphs and $G, H \in \mathcal{G}$. If $V(H) \subseteq V(G)$ and $E(H) \subseteq E(G)$, then we say that H is a *subgraph* of G and use the notation $H \subseteq G$. The number of subgraphs of G isomorphic to a fixed subgraph H is denoted by $\eta(G, H)$. It is easy to see that $\eta(G, S_2) = m$, the number of edges in G. The number of vertices of degree i in G will be denoted by $n_i = n_i(G)$. It is easy to see that $\sum_{i=1}^{\Delta(G)} n_i = |V(G)|$. A map Top from $\mathcal{G}$ into the set of all non-negative real numbers is called a *graph invariant* if $G \cong H$ implies that $Top(G) = Top(H)$. *Topological indices* are graph invariants applicable in chemistry.

The graph invariants *Wiener index* [14], *first Zagreb index* and *second Zagreb index* [9], *forgotten topological index* [6] and the *first general Zagreb index* [16], are defined as:

$$\begin{aligned}
W(G) &= \sum_{\{u,v\} \subset V(G)} d_G(u, v),\\
M_1(G) &= \sum_{v \in V(G)} deg_G(v)^2,\\
M_2(G) &= \sum_{uv \in E(G)} deg_G(u) deg_G(v),\\
F(G) &= \sum_{v \in V(G)} deg_G(v)^3 = \sum_{uv \in E(G)} [deg_G(u)^2 + deg_G(v)^2],\\
M_1^{\alpha}(G) &= \sum_{u \in V(G)} deg_G(u)^{\alpha},
\end{aligned}$$

respectively. Here, $\alpha \neq 0, 1$ is an arbitrary real number. Furthermore, the first Zagreb index and the forgotten topological index are just the case of $\alpha = 2, 3$ in the first general Zagreb index, respectively.

The first and second reformulated Zagreb indices of graphs were introduced by Milićević et al. [12]. These graph invariants are edge counterparts of the first and second Zagreb indices, respectively. These numbers can be defined as:

$$\begin{aligned}
EM_1(G) &= \sum_{e \sim f} [deg_G(e) + deg_G(f)] = \sum_{e \in E(G)} deg_G(e)^2,\\
EM_2(G) &= \sum_{e \sim f} deg_G(e) deg_G(f).
\end{aligned}$$

In this formulas, if $e = uv$ then $deg_G(e) = deg_G(u) + deg_G(v) - 2$. Moreover, $e \sim f$ means that the edges e and f are incident.

Suppose G is a simple graph with vertex set $\{v_1, \cdots, v_n\}$. The adjacency matrix of G is an $n \times n$ $0-1$ matrix $A = (a_{ij})$ such that a_{ij} is one if and only if there is an edge connecting v_i and v_j. The degree matrix, $D(G)$, is a square matrix of order n whose its i^{th} diagonal entry is equal to $deg_G(v_i)$ and whose off-diagonal elements are zero. The Laplacian matrix of G is defined as $L(G) = D(G) - A(G)$. The characteristic polynomial of the Laplacian matrix, $\psi(G, \lambda) = \det(\lambda I_n - L(G))$, is said to be the Laplacian polynomial of the graph G. In this paper we write this polynomial in the form of $\psi(G, \lambda) = \sum_{k=0}^{n}(-1)^{n-k}c_k(G)\lambda^k$. It is well-known that $c_k(G) \geq 0$, for all k.

Suppose G is a simple and undirected graph. The relationship between the coefficients of $\psi(G, \lambda)$ and the structure of G was established many years ago by Kel'mans [3, p. 38]. He proved that $c_k(G) = \sum_{F\in\mathcal{F}_k(G)}\gamma(F)$, where F is a spanning forest and the summation goes over the set $\mathcal{F}_k(G)$ of all spanning forests of G, possessing exactly k components and $\gamma(F)$ is the product of the number of vertices of the components of F. If T is an $n-$vertex tree, then for $k \geq 1$, the elements of $\mathcal{F}_k(T)$ can be obtained by deleting $k - 1$ distinct edges from T. So, it is easy to see that, $c_1(T) = n$, $c_n(T) = 1$ and $c_{n-1}(T) = 2(n - 1)$. Yan et al. [15], proved that $c_2(T) = W(T)$. Oliveira et al. [13], obtained closed formulas for the coefficient $c_{n-2}(T)$ and $c_{n-3}(T)$ in terms of the number of vertices, the first Zagreb and forgotten indices as $c_{n-2}(T) = 2n^2 - 5n + 3 - \frac{1}{2}M_1(T)$ and $c_{n-3}(T) = \frac{1}{3}[4n^3 - 18n^2 + 24n - 10 + F(T) - 3(n - 2)M_1(T)]$.

A matching K in a simple graph G is a set of pairwise non-adjacent edges, that is, no two edges of K share a common vertex. If $|K| = k$ then K is called a $k-$matching of G. The matching polynomial of G is a generating function for counting the number of $k-$matchings in G. Let $p(G, k)$ denote the number of $k-$matchings in G. Then the matching polynomial of G is defined as $M(G) = \sum_{k\geq 0}(-1)^k p(G, k)x^{n-2k}$, where $n = |V(G)|$. Farrell and Guo [5], established a formula for the number of $3-$matchings in terms of the size, degree sequence and number of triangles in given graph G, and Behmaram [2] continued this work to present a formula for the number of $4-$matchings of triangular-free graphs with respect to the number of vertices, edges, degrees and $4-$cycles.

2. Preliminary Results

The aim of this section is to state some results which are crucial throughout the paper. We encourage the interested readers to consult papers [1, 7] for more details.

The common vertex of two incident edges e and f is denoted by $e \cap f$. Define the graph invariants $\alpha(T)$ and $\beta(T)$ as follows:

$$\alpha(T) = \sum_{u\sim v} deg_T(u)deg_T(v)(deg_T(u) + deg_T(v)),$$

$$\beta(T) = \sum_{e\sim f} deg_T(e\cap f)(deg_T(e) + deg_T(f)).$$

Suppose T is a tree. In some of our results we need to have $\eta(T,H)$ for some special subgraphs of T. In the following lemma we record some cases which are important in our calculations. The following lemma is a restatement of Lemmas 2.1, 2.2 and 2.3 of [7] in which the number of paths of length 3, 4 and 5 are given.

LEMMA 2.1. *Let T be an $n-$vertex tree. Then,*

$$\eta(T,P_3) = \frac{1}{2}M_1(T) - n + 1,$$
$$\eta(T,P_4) = M_2(T) - M_1(T) + n - 1,$$
$$\eta(T,P_5) = EM_2(T) + EM_1(T) + \frac{3}{2}M_1(T) + \frac{1}{2}M_1^4(T) - \frac{3}{2}F(T) - n + 1 - \beta(T).$$

The number of stars with exactly four and five vertices in a given tree T are presented in the following lemma which is Lemma 2.2 in [1].

LEMMA 2.2. *Let T be an $n-$vrtex graph. Then,*

$$\eta(T,S_4) = \frac{1}{6}F(T) - \frac{1}{2}M_1(T) + \frac{2}{3}m,$$
$$\eta(T,S_5) = \frac{1}{24}M_1^4(T) - \frac{1}{4}F(T) + \frac{11}{24}M_1(T) - \frac{1}{2}m.$$

Let T be an arbitrary tree and $T_1, T_2, \ldots, T_5$ be graphs depicted in Figure 1. The number of subtrees of T isomorphic to one of these tress are given in the following lemma. These are restatements of Lemmas 2.3, 2.5., 2.7 and 2.15 in [1].

LEMMA 2.3. *Let T be an $n-vertex$ tree. Then we have,*

$$\eta(T,T_1) = n.\eta(T,P_4) + 2M_2(T) + F(T) - M_1(T) - 2\eta(T,P_5) - \alpha(T).$$
$$\eta(T,T_2) = \frac{1}{2}\alpha(T) + \frac{5}{2}M_1(T) - 3M_2(T) - \frac{1}{2}F(T) - 2m.$$
$$\eta(T,T_3) = \eta(T,P_3)(\frac{1}{2}M_1(T) - n - 3) - \frac{5}{4}M_1^4(T) + \frac{11}{2}F(T) + 6M_2(T) - \frac{33}{4}M_1(T) - 2EM_2(T) + 4m - \alpha(T) + 2\beta(T) - 3EM_1(T).$$
$$\eta(T,T_4) = \frac{1}{2}\eta(T,P_3)\Big((n+1)(n+2) - M_1(T) + 4\Big) + \frac{1}{4}(6n+52)M_1(T) - \frac{1}{4}(2n+36)F(T) + 2M_1^4(T) - (2n+9)M_2(T) + 3EM_2(T) - 8(n-1) + \frac{5}{2}\alpha(T) - 3\beta(T) + 5EM_1(T).$$
$$\eta(T,T_5) = (n+2)\eta(T,S_4) - \frac{1}{2}\alpha(T) + \frac{1}{2}F(T) + 3M_2(T) - \frac{1}{6}M_1^4(T) - \frac{4}{3}M_1(T).$$

In [1], the authors proved a useful formula for computing the $4-$matching of a tree which is important in our calculations.

THEOREM 2.4. *Let T be a tree with n vertices. Then,*

$$p(T,4) = \frac{1}{24}(n-1)(n^3+3n^2+22n+4) - \frac{1}{4}(n^2+5n+\frac{27}{6})M_1(T) + \frac{1}{4}M_1(T)^2 + (n+1)M_2(T) + \frac{1}{6}(2n+\frac{29}{2})F(T) - \frac{21}{24}M_1^4(T) - EM_2(T) - EM_1(T) + \beta(T) - \alpha(T) - \sum_{\{u,v\}\subset V(T)} \binom{deg_T(u)}{2}\binom{deg_T(v)}{2}.$$

LEMMA 2.5. *Let T be an $n-$vertex tree. Then*

$$\beta(T) - \alpha(T) = M_1^4(T) - 3F(T) + 2M_1(T) - 2M_2(T).$$

PROOF. By definition,

$$\begin{aligned}
\beta(T) &= \sum_{e\sim f, e=uv, f=vx} deg_T(v)(deg_T(e)+deg_T(f)) \\
&= \sum_{u\sim v\sim x} deg_T(v)\Big(deg_T(u)+deg_T(v)-2+deg_T(v)+deg_T(x)-2\Big) \\
&= 2\sum_{u\sim v\sim x} deg_T(v)^2 - 4\sum_{u\sim v\sim x} deg_T(v) + \sum_{u\sim v\sim x} deg_T(v)(deg_T(u)+deg_T(x)) \\
&= 2\sum_{v\in V(T)} \binom{deg_T(v)}{2} deg_T(v)^2 - 4\sum_{v\in V(T)}\binom{deg_T(v)}{2} deg_T(v) \\
&+ \sum_{uv\in E(T)} deg_T(u)deg_T(v)(deg_T(u)+deg_T(v)-2) \\
&= \sum_{v\in V(T)} (deg_T(v)^4 - deg_T(v)^3) - 2\sum_{v\in V(T)} (deg_T(v)^3 - deg_T(v)^2) \\
&- 2M_2(T) + \alpha(T).
\end{aligned}$$

Therefore, $\beta(T) - \alpha(T) = M_1^4(T) - 3F(T) + 2M_1(T) - 2M_2(T)$, which completes the proof. □

LEMMA 2.6. *Let T be a tree with n vertices. Then*

$$\eta(T,P_5) = 6n - \frac{1}{4}F(T) - \frac{39}{8}M_1(T) + \frac{1}{2}nM_1(T) - \frac{1}{8}(M_1(T))^2 - \frac{1}{2}n^2 + \frac{5}{8}M_1^4(T) + EM_2(T) + 3M_2(T) - \frac{11}{2} - \frac{1}{2}EM_1(T) - \beta(T) + \sum_{\{u,v\}\subset V(T)} \binom{deg_T(u)}{2}\binom{deg_T(v)}{2}.$$

PROOF. By definition,

$$\eta(T,P_5) = \binom{n-1}{4} - \Big(\eta(T,T_1) + \eta(T,T_2) + \eta(T,T_3) + \eta(T,T_4) + \eta(T,T_5) + \eta(T,S_5) + p(T,4)\Big).$$

Now, we apply Lemmas 2.2, 2.3, Theorem 2.4 and above discussion to deduce that

$$\begin{aligned}\eta(T,P_5) &= 6n-\frac{1}{4}F(T)-\frac{39}{8}M_1(T)+\frac{1}{2}nM_1(T)-\frac{1}{8}(M_1(T))^2-\frac{1}{2}n^2\\&+\frac{5}{8}M_1^4(T)+EM_2(T)+3M_2(T)-\frac{11}{2}-\frac{1}{2}EM_1(T)-\beta(T)\\&+\sum_{\{u,v\}\subset V(T)}\binom{deg_T(u)}{2}\binom{deg_T(v)}{2},\end{aligned}$$

proving the lemma. □

Lemma 2.7. *Let T be a tree with n vertices and $A(T)=\sum_{\{u,v\}\subset V(T)}\binom{deg_T(u)}{2}\binom{deg_T(v)}{2}$. Then*

$$\begin{aligned}A(T) &= \frac{3}{2}EM_1(T)+\frac{51}{8}M_1(T)-\frac{1}{8}M_1^4(T)-\frac{5}{4}F(T)-7n+\frac{13}{2}-\frac{1}{2}nM_1(T)\\&+\frac{1}{8}(M_1(T))^2+\frac{1}{2}n^2-3M_2(T).\end{aligned}$$

Proof. By two formulas for $\eta(T,P_5)$ given Lemmas 2.1, 2.6, and a simple calculation we have

$$\begin{aligned}A(T) &= \frac{3}{2}EM_1(T)+\frac{51}{8}M_1(T)-\frac{1}{8}M_1^4(T)-\frac{5}{4}F(T)-7n+\frac{13}{2}-\frac{1}{2}nM_1(T)\\&+\frac{1}{8}(M_1(T))^2+\frac{1}{2}n^2-3M_2(T),\end{aligned}$$

proving the lemma. □

Lemma 2.8. *Let G be a graph with m edges. Then $EM_1(T)=F(G)+2M_2(G)-4M_1(G)+4m$.*

Proof. By definition,

$$\begin{aligned}EM_1(T) &= \sum_{e=uv\in E(G)}deg_G(e)^2=\sum_{e=uv\in E(G)}(deg_G(u)+deg_G(v)-2)^2\\&=\sum_{e=uv\in E(G)}\Big(deg_G(u)^2+deg_G(v)^2+2deg_G(u)deg_G(v)\\&-4(deg_G(u)+deg_G(v))+4\Big)=F(G)+2M_2(G)-4M_1(T)+4m,\end{aligned}$$

as desired. □

Theorem 2.9. (*See* [1]) *Let T be a tree with n vertices. Then*

$$\begin{aligned} c_{n-4}(T) &= (n-1)(\frac{16}{24}n^3 - 4n^2 + \frac{348}{24}n - \frac{532}{6}) + \frac{17}{8}M_1(T)^2 \\ &\quad + (\frac{4}{6}n - \frac{412}{24})F(T) + \frac{39}{2}EM_1(T) - \frac{108}{48}M_1^4(T) - 40M_2(T) \\ &\quad - (n^2 + \frac{7}{2}n - \frac{1920}{24})M_1(T) - 16\sum_{\{u,v\}\subset V(T)} \binom{deg_T(u)}{2}\binom{deg_T(v)}{2}. \end{aligned}$$

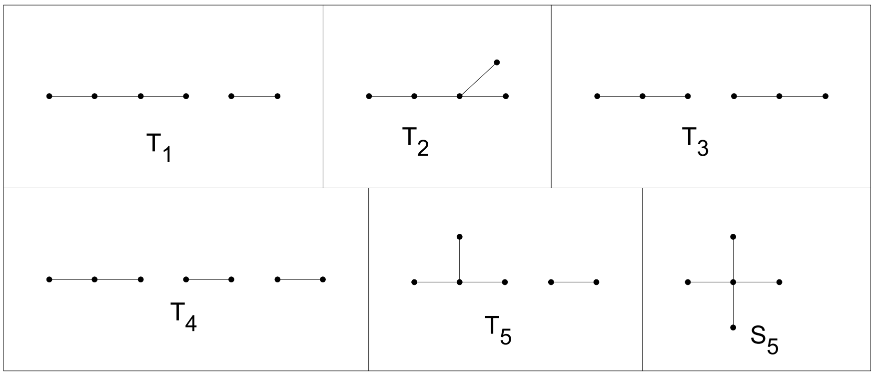

Figure 1. The graphs T_1, …, T_5 and S_5.

3. Main Results

Suppose T is a tree. It is well known that the Laplacian coefficient $c_{n-2}(T)$ is equal to the Wiener index of T, while $c_{n-3}(T)$ is equal to the modified hyper-Wiener index of T. We refer to [11] for more information on this topic. So, it is natural to think about the coefficient $c_{n-4}(T)$ and its relationship with some other topological indices of T.

The following environments are predefined:

Theorem 3.1. *Let T be a tree with n vertices. Then,*

$$\begin{aligned} p(T,4) &= \frac{1}{24}(n-1)(n^3+3n^2+10n-80) + \frac{1}{8}M_1(T)(-2n^2+M_1(T)-6n+36) \\ &\quad + M_2(T)(n-3) + \frac{1}{6}F(T)(2n-11) + \frac{1}{4}M_1^4(T) - EM_2(T). \end{aligned}$$

Proof. By Theorem 2.4,

$$p(T,4)=\frac{1}{24}(n-1)(n^3+3n^2+22n+4)-\frac{1}{4}(n^2+5n+\frac{27}{6})M_1(T)+\frac{1}{4}M_1(T)^2$$
$$+(n+1)M_2(T)+\frac{1}{6}(2n+\frac{29}{2})F(T)-\frac{21}{24}M_1^4(T)-EM_2(T)-EM_1(T)$$
$$+\beta(T)-\alpha(T)-\sum_{\{u,v\}\subset V(T)}\binom{deg_T(u)}{2}\binom{deg_T(v)}{2}.$$

Now, by Lemmas 2.5 and 2.7, we have

$$p(T,4)=\frac{1}{24}(n-1)(n^3+3n^2+10n+160)+\frac{1}{8}M_1(T)(-2n^2+M_1(T)-6n-44)$$
$$+M_2(T)(n+2)+\frac{1}{3}F(T)(n+2)+\frac{1}{4}M_1^4(T)-EM_2(T)-\frac{5}{2}EM_1(T),$$

and by Lemma 2.8,

$$p(T,4)=\frac{1}{24}(n-1)(n^3+3n^2+10n-80)+\frac{1}{8}M_1(T)(-2n^2+M_1(T)-6n+36)$$
$$+M_2(T)(n-3)+\frac{1}{6}F(T)(2n-11)+\frac{1}{4}M_1^4(T)-EM_2(T).$$

This completes the proof. □

Theorem 3.2. *Let T be a tree with n vertices. Then*

$$c_{n-4}(T)=\frac{1}{6}(n-1)(4n^3-24n^2+39n-16)+\frac{1}{3}F(G)(2n-5)$$
$$+\frac{1}{8}M_1(T)(-8n^2+M_1(T)+36n-32)-\frac{1}{4}M_1^4(T)-M_2(T).$$

Proof. By Lemmas 2.7, 2.8, Theorem 2.9, and simple calculations we have

$$c_{n-4}(T)=\frac{1}{6}(n-1)(4n^3-24n^2+39n-16)+\frac{1}{3}F(G)(2n-5)$$
$$+\frac{1}{8}M_1(T)(-8n^2+M_1(T)+36n-32)-\frac{1}{4}M_1^4(T)-M_2(T).$$

Hence the result. □

A pendant path of a graph G is a path P, in which one terminal vertex is of degree at least three, another terminal vertex is a pendant vertex, and all internal vertices (if any exists) are of degree two in G. It is clear that the number of pendant paths in G is equal to the number of pendant vertices in G. An internal path of G is a path I, in which two terminal vertices are of degree at least three and each internal vertex (if any exists) is of degree two in G. We also assume that α_i, $1 \leq i \leq 6$, are classes of chemical trees presented in Table 1.

Transformation *A***.** Suppose G is a chemical tree with two given pendant paths $P := v_1v_2\ldots v_k$ and $Q := u_1u_2\ldots u_l$ such that $k, l \geq 3$ and $deg_G(v_k) = deg_G(u_l) = 1$. Define $G' = G - v_2v_3 + v_3u_l$.

TABLE 1. Degree distributions of chemical trees with $2 \leq n_1(T) \leq 5$.

E.C.	n_4	n_3	n_2	n_1	E.C.	n_4	n_3	n_2	n_1
α_1	0	0	$n-2$	2	α_4	1	0	$n-5$	4
α_2	0	1	$n-4$	3	α_5	1	1	$n-7$	5
α_3	0	2	$n-6$	4	α_6	0	3	$n-8$	5

LEMMA 3.3. *Let G and G' be two chemical trees as described in Transformation A, with n (≥ 4) vertices. Then $c_{n-4}(G) < c_{n-4}(G')$.*

PROOF. By definitions of G and G', we have

$$M_1(G) = M_1(G'),\ F(G) = F(G'),\ M_1^4(G) = M_1^4(G').$$

Therefore by Theorem 3.2,

$$c_{n-4}(G) - c_{n-4}(G') = M_2(G') - M_2(G) = 2 - deg_G(v_1).$$

Now, $deg_G(v_1) \in \{3, 4\}$ and so, $c_{n-4}(G) - c_{n-4}(G') < 0$. □

Transformation B**.** Suppose G is a chemical tree with a given internal path $P_2 := v_1v_2$. In addition, we assume that $Q := u_1u_2 \ldots u_l$ is a pendant or internal path in G, such that $l \geq 4$. Define $G' = G - \{v_1v_2, u_1u_2, u_2u_3\} + \{v_1u_2, u_2v_2, u_1u_3\}$.

LEMMA 3.4. *Let G and G' be two chemical trees as described in Transformation B, with n (≥ 8) vertices. Then $c_{n-4}(G) < c_{n-4}(G')$.*

PROOF. By definitions of G and G', $M_1(G) = M_1(G')$, $F(G) = F(G')$ and $M_1^4(G) = M_1^4(G')$. We now apply Theorem 3.2 to deduce that $c_{n-4}(G) - c_{n-4}(G') = M_2(G') - M_2(G) = 2deg_G(v_1) + 2deg_G(v_1) - deg_G(v_1)deg_G(v_2) - 4$. Therefore, $deg_G(v_1), deg_G(v_2) \in \{3, 4\}$ and so $c_{n-4}(G) - c_{n-4}(G') < 0$. □

Transformation C**.** Suppose G is a chemical tree with a given pendant path $P_2 := v_1v_2 \ldots v_k$ such that $k \geq 3$ and $deg_G(v_k) = 1$. In addition, we assume that $Q := u_1u_2 \ldots u_l$ is an internal path in G, such that $l \geq 3$. Define $G' = G - \{v_2v_3, u_1u_2\} + \{u_1v_3, v_ku_2\}$.

LEMMA 3.5. *Let G_1 and G_2 be two chemical trees as explained in Transformation C, with n (≥ 8) vertices. Then $c_{n-4}(G) < c_{n-4}(G')$.*

PROOF. By definitions of G and G', $M_1(G) = M_1(G')$, $F(G) = F(G')$ and $M_1^4(G) = M_1^4(G')$. Apply Theorem 3.2 to prove that $c_{n-4}(G) - c_{n-4}(G')$ $= M_2(G') - M_2(G) = 4 + deg_G(v_1) - [2 + 2deg_G(v_1)] = 2 - deg_G(v_1)$. Since $deg_G(v_1) \in \{3, 4\}$, $c_{n-4}(G) - c_{n-4}(G') < 0$. □

Transformation D**.** Suppose G is a chemical tree with two given pendant paths $P := v_1v_2\dots v_k$ and $Q := u_1u_2\dots u_l$ such that $deg_G(v_k) = deg_G(u_l) = 1$. Define $G' = G - v_1v_2 + u_lv_2$.

Let T be a tree on n vertices. Then Gutman and Das in [10] have proved that

$$M_1(T) \leq n(n-1), \tag{3.1}$$

with equality if and only if $T \cong S_n$.

LEMMA 3.6. *Let G and G' be two chemical trees as in Transformation D, with n (≥ 8) vertices. Then $c_{n-4}(G) < c_{n-4}(G')$.*

PROOF. By definitions, if $deg_G(v_1) = 3$, then

$$M_1(G) = M_1(G') + 2,\ F(G) = F(G') + 12,\ M_1^4(G) = M_1^4(G') + 50.$$

Therefore, by Theorem 3.2 and a simple calculation we have,

$$c_{n-4}(G) - c_{n-4}(G') \geq \frac{1}{2}M_1(G) - 2n^2 + 17n - 41 - M_2(G) + M_2(G').$$

By Equation (3), $M_1(G) \leq n(n-1)$ and so,

$$c_{n-4}(G) - c_{n-4}(G') \leq \frac{1}{2}(33n - 3n^2) - 41 - M_2(G) + M_2(G').$$

Next by [4, Lemma 2.1], $M_2(G') \leq M_2(G)$. This proves that

$$c_{n-4}(G) - c_{n-4}(G') \leq \frac{1}{2}(33n - 3n^2) - 41 < 0.$$

The proof of the case that $deg_G(v_1) = 4$, is similar. □

LEMMA 3.7. [8, Lemma 2.3] *If T is a chemical tree with n vertices, then*

$$n_1(T) = 2 + n_3(T) + 2n_4(T) \text{ and } n_2(T) = n - [2 + 2n_3(T) + 3n_4(T)].$$

LEMMA 3.8. *There exists a chemical tree of order n with $2 \leq n_1(T) \leq 5$, if and only if T belongs to one of the equivalence classes ($E.C.$) given in Table 1.*

PROOF. We distinguish the following four cases:

1. $n_1(T) = 2$.
2. $n_1(T) = 3$.
3. $n_1(T) = 4$.
4. $n_1(T) = 5$.

To prove case (1), let $n_1(T) = 2$. Then by Lemma 3.7, there is a tree T with $n_1(T) = 2$ if and only if $n_3(T) + 2n_4(T) = 0$, if and only if $n_3(T) = n_4(T) = 0$ if and only if $n_2(T) = n - 2$ if and only if $T \in \alpha_1$. The proofs of the other cases are similar and we omit them. □

The number of edges connecting vertices of degree i and j in a graph A is denoted by $m_{i,j}(A)$. For a positive integer $n \geq 10$, we define:

$B_1 = \{T \in \alpha_5 \mid m_{1,3}(T) = 2, m_{1,4}(T) = 3, m_{2,3}(T) = m_{2,4}(T) = 1, m_{2,2}(T) = n - 8\}$.

$B_2 = \{T \in \alpha_6 :\ m_{1,3}(T) = 5,\ m_{2,3}(T) = 4,\ \textit{and}\ m_{2,2}(T) = n - 10\}$.

By Theorem 3.2, it is easy to see that for each $T \in B_1$ and $T' \in B_2$ we have

$$c_{n-4}(T) = \frac{1}{6}(2n-9)(2n^3 - 17n^2 + 25n + 86), \tag{3.2}$$

$$c_{n-4}(T') = \frac{2}{3}n^4 - \frac{26}{3}n^3 + \frac{215}{6}n^2 - \frac{191}{6}n - 63. \tag{3.3}$$

LEMMA 3.9. *Let T be a chemical tree with $n_1(T) \geq 5$. Then,*

$$c_{n-4}(T) \leq \frac{2}{3}n^4 - \frac{26}{3}n^3 + \frac{215}{6}n^2 - \frac{191}{6}n - 63,$$

with equality if and only if $T \in B_2$.

PROOF. If $n_1(T) = 5$, then Lemmas 3.3, 3.4, 3.5, 3.8, and Equations 3.2, 3.3 give us the result. If $n_1(T) \geq 6$, then by repeated application of Transformation D we obtain a tree, say T', such that $n_1(T') = 5$, and by Lemma 3.6, $c_{n-4}(T') > c_{n-4}(T)$. But $c_{n-4}(T') \leq \frac{2}{3}n^4 - \frac{26}{3}n^3 + \frac{215}{6}n^2 - \frac{191}{6}n - 63$, proving the lemma. □

We now apply Lemma 3.8 and Theorem 3.2, to compute the coefficient c_{n-4} for all chemical trees with $n \geq 10$ vertices and $2 \leq n_1 \leq 4$.

$A_1 = \{T \in \alpha_1 \mid m_{1,2}(T) = 2, m_{2,2}(T) = n - 3\}$,
$A_2 = \{T \in \alpha_2 \mid m_{1,2}(T) = 1, m_{1,3}(T) = 2, m_{2,3}(T) = 1, m_{2,2}(T) = n - 5\}$,
$A_3 = \{T \in \alpha_2 \mid m_{1,2}(T) = 2, m_{1,3}(T) = 1, m_{2,3}(T) = 2, m_{2,2}(T) = n - 6\}$,
$A_4 = \{T \in \alpha_2 \mid m_{1,2}(T) = 3, m_{2,3}(T) = 3, m_{2,2}(T) = n - 7\}$,
$A_5 = \{T \in \alpha_3 \mid m_{1,3}(T) = 4, m_{2,3}(T) = 2, m_{2,2}(T) = n - 7\}$,
$A_6 = \{T \in \alpha_3 \mid m_{1,2}(T) = 1, m_{1,3}(T) = 3, m_{2,3}(T) = 3, m_{2,2}(T) = n - 8\}$,
$A_7 = \{T \in \alpha_3 \mid m_{1,2}(T) = 2, m_{1,3}(T) = 2, m_{2,3}(T) = 4, m_{2,2}(T) = n - 9\}$,
$A_8 = \{T \in \alpha_3 \mid m_{1,2}(T) = 3, m_{1,3}(T) = 1, m_{2,3}(T) = 5, m_{2,2}(T) = n - 10\}$,
$A_9 = \{T \in \alpha_3 \mid m_{1,2}(T) = 4, m_{2,3}(T) = 6, m_{2,2}(T) = n - 11\}$,
$A_{10} = \{T \in \alpha_3 \mid m_{1,2}(T) = m_{2,3}(T) = m_{3,3}(T) = 1, m_{1,3}(T) = 3, m_{2,2}(T) = n - 7\}$,
$A_{11} = \{T \in \alpha_3 \mid m_{1,2}(T) = m_{1,3}(T) = m_{2,3}(T) = 2, m_{3,3}(T) = 1, m_{2,2}(T) = n - 8\}$,
$A_{12} = \{T \in \alpha_3 \mid m_{1,2}(T) = m_{2,3}(T) = 3, m_{1,3}(T) = m_{3,3}(T) = 1, m_{2,2}(T) = n - 9\}$,
$A_{13} = \{T \in \alpha_3 \mid m_{1,2}(T) = 4, m_{2,3}(T) = 4, m_{3,3}(T) = 1, m_{2,2}(T) = n - 10\}$,
$A_{14} = \{T \in \alpha_4 \mid m_{1,2}(T) = 1, m_{1,4}(T) = 3, m_{2,4}(T) = 1, m_{2,2}(T) = n - 6\}$,
$A_{15} = \{T \in \alpha_4 \mid m_{1,2}(T) = 2, m_{1,4}(T) = 2, m_{2,4}(T) = 2, m_{2,2}(T) = n - 7\}$,
$A_{16} = \{T \in \alpha_4 \mid m_{1,2}(T) = 3, m_{1,4}(T) = 1, m_{2,4}(T) = 3, m_{2,2}(T) = n - 8\}$,
$A_{17} = \{T \in \alpha_4 \mid m_{1,2}(T) = 4, m_{2,4}(T) = 4, m_{2,2}(T) = n - 9\}$.

Let $T_i \in A_i$, for $i = 1, 2, \dots, 17$. Then by Theorem 3.2, we have:

$$\begin{aligned}
c_{n-4}(T_1) &= \frac{1}{6}(2n-5)(2n-7)(n-3)(n-4),\\
c_{n-4}(T_2) &= \frac{2}{3}n^4 - \frac{26}{3}n^3 + \frac{239}{6}n^2 - \frac{419}{6}n + 25,\\
c_{n-4}(T_3) &= \frac{1}{6}(2n-9)(2n^3 - 17n^2 + 43n - 16),\\
c_{n-4}(T_4) &= \frac{2}{3}n^4 - \frac{26}{3}n^3 + \frac{239}{6}n^2 - \frac{419}{6}n + 23,\\
c_{n-4}(T_5) &= \frac{2}{3}n^4 - \frac{26}{3}n^3 + \frac{227}{6}n^2 - \frac{305}{6}n - 19,\\
c_{n-4}(T_6) &= \frac{2}{3}n^4 - \frac{26}{3}n^3 + \frac{227}{6}n^2 - \frac{305}{6}n - 20,\\
c_{n-4}(T_7) &= c_{n-4}(T_{10}) = \frac{1}{6}(2n-9)(2n^3 - 17n^2 + 37n + 14),\\
c_{n-4}(T_8) &= c_{n-4}(T_{11}) = \frac{2}{3}n^4 - \frac{26}{3}n^3 + \frac{227}{6}n^2 - \frac{305}{6}n - 22,\\
c_{n-4}(T_9) &= c_{n-4}(T_{12}) = \frac{2}{3}n^4 - \frac{26}{3}n^3 + \frac{227}{6}n^2 - \frac{305}{6}n - 23,\\
c_{n-4}(T_{13}) &= \frac{2}{3}n^4 - \frac{26}{3}n^3 + \frac{227}{6}n^2 - \frac{305}{6}n - 24,\\
c_{n-4}(T_{14}) &= \frac{2}{3}n^4 - \frac{26}{3}n^3 + \frac{215}{6}n^2 - \frac{167}{6}n - 87,\\
c_{n-4}(T_{15}) &= \frac{2}{3}n^4 - \frac{26}{3}n^3 + \frac{215}{6}n^2 - \frac{167}{6}n - 89,\\
c_{n-4}(T_{16}) &= \frac{2}{3}n^4 - \frac{26}{3}n^3 + \frac{215}{6}n^2 - \frac{167}{6}n - 91,\\
c_{n-4}(T_{17}) &= \frac{2}{3}n^4 - \frac{26}{3}n^3 + \frac{215}{6}n^2 - \frac{167}{6}n - 93,
\end{aligned} \tag{3.4}$$

Theorem 3.10. *If $n \geq 11$, $T_i \in A_i$, for $i = 1, 2, \dots, 17$, $T_{18} \in B_2$, and $T \in \mathcal{CT}(n) \setminus \{T_1, T_2, \dots, T_{18}\}$, then* $c_{n-4}(T_1) > c_{n-4}(T_2) > c_{n-4}(T_3) > c_{n-4}(T_4) > c_{n-4}(T_5) > c_{n-4}(T_6) > c_{n-4}(T_7) = c_{n-4}(T_{10}) > c_{n-4}(T_8) = c_{n-4}(T_{11}) > c_{n-4}(T_9) = c_{n-4}(T_{12}) > c_{n-4}(T_{13}) > c_{n-4}(T_{14}) > c_{n-4}(T_{15}) > c_{n-4}(T_{16}) > c_{n-4}(T_{17}) > c_{n-4}(T_{18}) > c_{n-4}(T)$.

Proof. By Equations 3.3 and 3.4, $c_{n-4}(T_1) > c_{n-4}(T_2) > c_{n-4}(T_3) > c_{n-4}(T_4) > c_{n-4}(T_5) > c_{n-4}(T_6) > c_{n-4}(T_7) = c_{n-4}(T_{10}) > c_{n-4}(T_8) = c_{n-4}(T_{11}) > c_{n-4}(T_9) = c_{n-4}(T_{12}) > c_{n-4}(T_{13}) > c_{n-4}(T_{14}) > c_{n-4}(T_{15}) > c_{n-4}(T_{16}) > c_{n-4}(T_{17}) > c_{n-4}(T_{18})$. Since $T \notin \{T_1, T_2, \dots, T_{18}\}$, $n_1(T) \geq 5$ and Lemma 3.9, gives the result. ∎

Remark 3.11. 1. If $n = 10$, then $c_{n-4}(T_1) > c_{n-4}(T_2) > c_{n-4}(T_3) > c_{n-4}(T_4) > c_{n-4}(T_5) > c_{n-4}(T_6) > c_{n-4}(T_7) = c_{n-4}(T_{10}) > c_{n-4}(T_8)$

$= c_{n-4}(T_{11}) > c_{n-4}(T_{12}) > c_{n-4}(T_{13}) > c_{n-4}(T_{14}) > c_{n-4}(T_{15}) > c_{n-4}(T_{16}) > c_{n-4}(T_{17}) > c_{n-4}(T_{18}) > c_{n-4}(T)$.

2. If $n = 9$, then $c_{n-4}(T_1) > c_{n-4}(T_2) > c_{n-4}(T_3) > c_{n-4}(T_4) > c_{n-4}(T_5) > c_{n-4}(T_6) > c_{n-4}(T_7) = c_{n-4}(T_{10}) > c_{n-4}(T_{11}) > c_{n-4}(T_{12}) > c_{n-4}(T_{14}) > c_{n-4}(T_{15}) > c_{n-4}(T_{16}) > c_{n-4}(T_{17}) > c_{n-4}(T)$.
3. If $n = 8$, then $c_{n-4}(T_1) > c_{n-4}(T_2) > c_{n-4}(T_3) > c_{n-4}(T_4) > c_{n-4}(T_5) > c_{n-4}(T_6) > c_{n-4}(T_{10}) > c_{n-4}(T_{11}) > c_{n-4}(T_{14}) > c_{n-4}(T_{15}) > c_{n-4}(T_{16}) > c_{n-4}(T)$.
4. If $n = 7$, then $c_{n-4}(T_1) > c_{n-4}(T_2) > c_{n-4}(T_3) > c_{n-4}(T_4) > c_{n-4}(T_5) > c_{n-4}(T_{10}) > c_{n-4}(T_{14}) > c_{n-4}(T_{15}) > c_{n-4}(T)$.
5. If $n = 6$, then $c_{n-4}(T_1) > c_{n-4}(T_2) > c_{n-4}(T_3) > c_{n-4}(T_{14}) > c_{n-4}(T)$.
6. If $n = 5$, then $c_{n-4}(T_1) = c_{n-4}(T_2) = c_{n-4}(S_5)$.

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References

[1] A. R. Ashrafi, M. Eliasi and A. Ghalavand, *Laplacian coefficients and Zagreb indices of trees*, Linear Multilinear Algebra **67**(9) (2019), 1736–1749.

[2] A. Behmaram, *On the number of 4-matchings in graphs*, MATCH Commun. Math. Comput. Chem. **62** (2009), 381–388.

[3] D. Cvetković, M. Doob and H. Sachs, *Spectra of Graphs – Theory and Application*, Barth, Heidelberg, 1995.

[4] M. Eliasi and A. Ghalavand, *Trees with the Minimal Second Zagreb Index*, Kragujevac J. Math. **42**(3) (2018), 325–333.

[5] E. J. Farrell and J. M. Guo, *On matching coefficients*, Discrete Math. **89** (1991), 203–210.

[6] B. Furtula and I. Gutman, *A forgotten topological index*, J. Math. Chem. **53** (2015), 1184–1190.

[7] A. Ghalavand, M. Eliasi and A. R. Ashrafi, *Relations between Wiener, hyper-Wiener and some Zagreb type indices*, Kragujevac J. Sci. **41** (2019), 37–42.

[8] I. Gutman, A. Ghalavand, T. Dehghan-Zadeh and A. R. Ashrafi, *Graphs with smallest forgotten index*, Iranian J. Math. Chem. **8** (3) (2017), 259–273.

[9] I. Gutman and N. Trinajstić, *Graph theory and molecular orbitals. Total $\pi-$electron energy of alternant hydrocarbons*, Chem. Phys. Lett. **17** (1972), 535–538.

[10] I. Gutman and K. Ch. Das, *The first Zagreb indices* 30 *years after*, MATCH Commun. Math. Comput. Chem. **50** (2004), 83–92.

[11] A. Ilić, *Trees with minimal Laplacian coefficients*, Comput. Math. Appl. **59** (8) (2010), 2776–2783.

[12] A. Milićević, S. Nikolić and N. Trinajstić, *On reformulated Zagreb indices*, Mol. Divers. **8** (2004), 393–399.

[13] C. S. Oliveira, N. M. M. de Abreu, S. Jurkewicz, *The characteristic polynomial of the Laplacian of graphs in $(a, b)-$linear classes*, Linear Algebra Appl. **356** (2002) 113–121.

[14] H. Wiener, *Structural determination of paraffin boiling points*, J. Am. Chem. Soc. **69** (1947) 17–20.

[15] W. Yan and Y.-N. Yeh, *Connections between Wiener index and matchings*, J. Math. Chem. **39** (2006) 389–399.

[16] S. Zhang and H. Zhang, *Unicyclic graphs with the first three smallest and largest first general Zagreb index*, MATCH Commun. Math. Comput. Chem. **55** (2) (2006), 427–438.

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