BULLETIN OF THE INTERNATIONAL MATHEMATICAL VIRTUAL INSTITUTE
ISSN (p) 2303-4874, ISSN (o) 2303-4955
www.imvibl.org /JOURNALS / BULLETIN
Vol. 8(2018), 369-383
DOI: 10.7251/BIMVI1802369G

Former
BULLETIN OF THE SOCIETY OF MATHEMATICIANS BANJA LUKA
ISSN 0354-5792 (o), ISSN 1986-521X (p)

EXTREMAL GRAPHS FOR THE SECOND MULTIPLICATIVE ZAGREB INDEX

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Abstract. Let G be a graph with edge set $E(G)$. The second multiplicative Zagreb index of G is defined as $\Pi_2(G) = \prod_{uv\in E(G)}[deg_G(u)\, deg_G(v)]$, where $deg_G(v)$ is the degree of the vertex v of G. In this paper, the unicyclic graphs with first through seventh smallest Π_2-values are determined, and the same is done for the first through eighth bicyclic, tetracyclic, and pentacyclic graphs, respectively, and the first through eleventh tricyclic graphs. In addition, we identify the eighth classes of chemical trees, with the first through eighth smallest Π_2-values among all connected graphs of order $n \geqslant 10$. This extendsq the results of an earlier paper on this topic.

1. Introduction

Throughout this paper all graphs are assumed to be connected, undirected and simple. Let G be such a graphs, with vertex set $V(G)$ and edge set $E(G)$. We use the usual notation uv for an edge connecting the vertices u and v in a graph G, and $N[v, G]$ for the set of all vertices adjacent to v, i.e., $N[v, G] = \{t \in V(G) \mid vt \in E(G)\}$. The degree of a vertex v is $deg_G(v) = |N[v, G]|$. The symbols $\Delta = \Delta(G)$ and $\delta = \delta(G)$, respectively, are used for the maximum and minimum degree of the vertices in G. A vertex of degree 1 is called a *pendent vertex*. The number of vertices of degree i will be denoted by n_i. One can easily seen that $\sum\limits_{i\geqslant 1} n_i = |V(G)|$. If the graph G has exactly n vertices, m edges and k components, then $c = m - n + k$ is its *cyclomatic number*. If $c = 1, 2, 3, 4, 5$, then the graph G is said to be unicyclic, bicyclic, tricyclic, tetracyclic, and pentacyclic, respectively.

2010 *Mathematics Subject Classification.* Primary 05C07; Secondary 05C35.
Key words and phrases. Degree (of vertex), Zagreb index, multiplicative Zagreb index.
The research of the first two authors was partially supported by the University of Kashan under grant no 364988/179.

Choose an edge e and non-adjacent vertices u, v in G. The subgraph of G obtained by removing the edge e is denoted by $G - e$. Moreover, $G + uv$ denotes the graph constructed from G by adding an edge uv. A tree in which all vertex degrees are at most four is called a *chemical tree* and the set of all n-vertex chemical trees will be denoted by $\tau(n)$. The notations P_n and S_n are used for the path star graphs n vertices, respectively.

2. Second Zagreb and Multiplicative Zagreb Indices of graphs

A real number λ which is invariant under graph isomorphism is said to be a *graph invariant*. A graph invariant applicable in chemistry is said to be a *topological index*. The *first* and *second Zagreb indices* of a given graph G are defined as

$$M_1(G) = \sum_{v \in V(G)} deg_G(v)^2 \quad \text{and} \quad M_2(G) = \sum_{uv \in E(G)} deg_G(u)\, deg_G(v)\,.$$

They were introduced as early as in the 1970s [**11, 10**] and were used to approximate the total π-electron energy and the molecular branching. Since then, M_1 and M_2 became one of the most thoroughly investigated degree–based topological indices [**8, 14**], whose mathematical properties have been studied in full detail [**1**].

The multiplicative variant of the first Zagreb index, namely $\prod\limits_{v \in V(G)} \deg_G(v)^2$, was proposed by Todeschini et al. [**17, 16**]. It was immediately noticed [**7**] that it is just the square of a much older topological index [**13**] that nowadays is usually referred to as the *Narumi–Katayama index*. The second multiplicative Zagreb index is defined as

$$\Pi_2(G) = \prod_{uv \in E(G)} deg_G(u)\, deg_G(v)\,.$$

Of the numerous recent studies of the second multiplicative Zagreb index, we mention the following. Liu and Zhang [**12**] established sharp upper bounds for Π_2 in terms of graph parameters such as order, size, and the first Zagreb index. They proved that if G is a nontrivial connected graph of order n and size m, then $\Pi_2(G) \leqslant \left(\frac{M_1(G)}{2m}\right)^{2m}$ with equality if and only if G is $\frac{2m}{n}$-regular. Yan and Liu [**20**] gave sharp upper and lower bounds for Π_2 of unicyclic graphs with n vertices and k pendent vertices. Xu and Hua [**19**] introduced several graph operations that increase Π_2. They applied this result to determine extremal (minimum and maximum) trees, unicyclic graphs, and bicyclic graphs with respect to Π_2. Wang et al. [**18**], characterized the bipartite graphs with the largest, second–largest and Π_2-values. Braun et al. [**2**] compared the similarity of 608 molecular descriptors, including Π_2. We encourage to the interested readers to consult papers [**3, 4, 6, 15, 19**] and the references cited therein for more information on this topic.

In the paper [**5**], the classes of trees (of a fixed order $n \geqslant 14$), with the first through eighth smallest multiplicative second Zagreb indices were characterized. Continuing these studies, we now report analogous results for (connected) graphs with cyclomatic number $c = 1, 2, 3, 4, 5$. In particular, we determine the first through seventh classes of unicyclic graphs with smallest Π_2-values, as well as the first through eighth such classes for bicyclic, tetracyclic, and pentacyclic graphs, and the first through eleventh such classes for tricyclic graphs. In addition, we identify the eighth classes of chemical trees, with the first through eighth smallest Π_2-values among all connected graphs of order $n \geqslant 10$. This generalizes the main result of [**5**] to all connected graphs.

It was shown in [**4**] that

$$\Pi_2(G) = \prod_{v \in V(G)} deg_G(v)^{deg_G(v)} . \tag{2.1}$$

We apply this equation to prove the following lemma:

Lemma 2.1. *Suppose that G is a graph and u_1, u_2 and u_3 are vertices of G, such that u_1u_2 is a cut edge, $deg_G(u_1) \geqslant 3$, $deg_G(u_3) = 1$, and u_2 is not on the path joining u_1 and u_3. If $G' = G - u_1u_2 + u_2u_3$, then $\Pi_2(G') < \Pi_2(G)$.*

Proof. By Equation 2.1 and the definition of G and G', we have

$$\begin{aligned} \frac{\Pi_2(G)}{\Pi_2(G')} &= \frac{deg_G(u_1)^{deg_G(u_1)} deg_G(u_3)^{deg_G(u_3)}}{deg_{G'}(u_1)^{deg_{G'}(u_1)} deg_{G'}(u_3)^{deg_{G'}(u_3)}} \\ &= \frac{deg_G(u_1)^{deg_G(u_1)}}{4 deg_{G'}(u_1)^{deg_{G'}(u_1)}} = \frac{deg_G(u_1)^{deg_G(u_1)}}{4(deg_G(u_1)-1)^{deg_G(u_1)-1}} \\ &> \frac{deg_G(u_1)^2}{4(deg_G(u_1)-1)} \geqslant \frac{3^2}{4 \times 2} > 1 . \end{aligned}$$

□

Lemma 2.2. *Suppose that G is a cyclic graph with given vertices u and v, such that uv is not a cut edge in G. If $G' = G - uv$, then $\Pi_2(G') < \Pi_2(G)$.*

Proof. By Equation 2.1 and the definition of G and G', we have

$$\begin{aligned} \frac{\Pi_2(G)}{\Pi_2(G')} &= \frac{deg_G(u)^{deg_G(u)} deg_G(v)^{deg_G(v)}}{deg_{G'}(u)^{deg_{G'}(u)} deg_{G'}(v)^{deg_{G'}(v)}} \\ &= \frac{deg_G(u)^{deg_G(u)} deg_G(v)^{deg_G(v)}}{(deg_G(u)-1)^{deg_G(u)-1} (deg_G(v)-1)^{deg_G(v)-1}} > 1 . \end{aligned}$$

□

3. Extremal graphs with respect to the second Zagreb index

In this section, we use arguments similar as in [**5, 9**], by means of which we determine the extremal values of the second multiplicative Zagreb index in the class of all (connected) unicyclic, bicyclic, tricyclic, tetracyclic, and pentacyclic graphs.

Lemma 3.1. *If G is a connected graph with n vertices and cyclomatic number c, then*

$$n_1(G) = 2 - 2c + \sum_{i=3}^{\Delta(G)} (i-2)n_i \quad \textit{and} \quad n_2(G) = 2c + n - 2 - \sum_{i=3}^{\Delta(G)} (i-1)n_i .$$

PROOF. We have $n_1 + n_2 + \sum_{i=3}^{\Delta(T)} n_i = n$ and $n_1 + 2n_2 + \sum_{i=3}^{\Delta(T)} n_i i = 2|E(G)| = 2(c+n-1)$. These equations give use the result. □

The following lemma is a consequence of Lemma 3.1.

COROLLARY 3.1. *There is a connected unicyclic graph G of order n with $n_1(G) \leqslant 4$ if and only if G belongs to one of equivalence classes given in Table 1.*

TABLE 1. Degree distributions of the connected unicyclic graphs with $n_1 \leqslant 4$ and $n_i = 0$ for $i \geqslant 7$.

E.C.	n_6	n_5	n_4	n_3	n_2	n_1	n_i	Π_2
A_1	0	0	0	0	n	0	0	$16777216 \times 2^{2(n-12)}$
A_2	0	0	0	1	$n-2$	1	0	$28311552 \times 2^{2(n-12)}$
A_3	0	0	1	0	$n-3$	2	0	$67108864 \times 2^{2(n-12)}$
A_4	0	0	0	2	$n-4$	2	0	$47775744 \times 2^{2(n-12)}$
A_5	0	0	0	3	$n-6$	3	0	$80621568 \times 2^{2(n-12)}$
A_6	0	0	1	1	$n-5$	3	0	$113246208 \times 2^{2(n-12)}$
A_7	0	1	0	0	$n-4$	3	0	$204800000 \times 2^{2(n-12)}$
A_8	0	0	0	4	$n-8$	4	0	$136048896 \times 2^{2(n-12)}$
A_9	0	0	1	2	$n-7$	4	0	$191102976 \times 2^{2(n-12)}$
A_{10}	0	0	2	0	$n-6$	4	0	$268435456 \times 2^{2(n-12)}$
A_{11}	0	1	0	1	$n-6$	4	0	$345600000 \times 2^{2(n-12)}$
A_{12}	1	0	0	0	$n-5$	4	0	$764411904 \times 2^{2(n-12)}$

PROOF. It is easy to see that $n_1(G) = 0, 1, 2, 3, 4$. Now a similar argument as in Corollary 2.7 in [**9**] proves the lemma. □

COROLLARY 3.2. *There is a connected bicyclic graph G of order n with $n_1(G) \leqslant 3$ if and only if G belongs to one of equivalence classes given in Table 2.*

PROOF. We have to note that there are four different classes in which $n_1(G) = 0, 1, 2, 3$. We now obtain the result by an argument similar to the proof of Corollary 2.10 in [**9**]. □

COROLLARY 3.3. *There is a connected tricyclic graph G of order n with $n_1(G) \leqslant 3$ if and only if G belongs to one of equivalence classes given in Tables 3, 4, 5, and 6.*

PROOF. We have exactly four cases for $n_1(G)$. These are $n_1(G) = 0, 1, 2, 3$. The proof follows from a similar argument as the proof of Corollary 2.13 in [**9**]. □

COROLLARY 3.4. *There is a connected tetracyclic graph G of order n with $n_1(G) \leqslant 2$ if and only if G belongs to one of the equivalence classes given in Tables 7, 8, and 9.*

TABLE 2. Degree distributions of the connected bicyclic graphs with $n_1 \leqslant 3$ and $n_i = 0$ for $i \geqslant 8$.

E.C.	n_7	n_6	n_5	n_4	n_3	n_2	n_1	n_i	Π_2
B_1	0	0	0	1	0	$n-1$	0	0	$1073741824 \times 2^{2(n-12)}$
B_2	0	0	0	0	2	$n-2$	0	0	$764411904 \times 2^{2(n-12)}$
B_3	0	0	1	0	0	$n-2$	1	0	$3276800000 \times 2^{2(n-12)}$
B_4	0	0	0	1	1	$n-3$	1	0	$1811939328 \times 2^{2(n-12)}$
B_5	0	0	0	0	3	$n-4$	1	0	$1289945088 \times 2^{2(n-12)}$
B_6	0	0	0	0	4	$n-6$	2	0	$2176782336 \times 2^{2(n-12)}$
B_7	0	0	0	1	2	$n-5$	2	0	$3057647616 \times 2^{2(n-12)}$
B_8	0	0	1	0	1	$n-4$	2	0	$5529600000 \times 2^{2(n-12)}$
B_9	0	0	0	2	0	$n-4$	2	0	$4294967296 \times 2^{2(n-12)}$
B_{10}	0	1	0	0	0	$n-3$	2	0	$12230590464 \times 2^{2(n-12)}$
B_{11}	0	0	0	0	5	$n-8$	3	0	$3673320192 \times 2^{2(n-12)}$
B_{12}	0	0	0	1	3	$n-7$	3	0	$5159780352 \times 2^{2(n-12)}$
B_{13}	0	0	1	0	2	$n-6$	3	0	$9331200000 \times 2^{2(n-12)}$
B_{14}	0	0	0	2	1	$n-6$	3	0	$7247757312 \times 2^{2(n-12)}$
B_{15}	0	1	0	0	1	$n-5$	3	0	$20639121408 \times 2^{2(n-12)}$
B_{16}	0	0	1	1	0	$n-5$	3	0	$13107200000 \times 2^{2(n-12)}$
B_{17}	1	0	0	0	0	$n-4$	3	0	$53971714048 \times 2^{2(n-12)}$

TABLE 3. Degree distributions of the connected tricyclic graphs with $n_1 = 0$ and $n_i = 0$ for $i \geqslant 7$.

E.C.	n_6	n_5	n_4	n_3	n_2	n_1	n_i	Π_2
D_1	1	0	0	0	$n-1$	0	0	$195689447424 \times 2^{2(n-12)}$
D_2	0	1	0	1	$n-2$	0	0	$88473600000 \times 2^{2(n-12)}$
D_3	0	0	2	0	$n-2$	0	0	$68719476736 \times 2^{2(n-12)}$
D_4	0	0	1	2	$n-3$	0	0	$48922361856 \times 2^{2(n-12)}$
D_5	0	0	0	4	$n-4$	0	0	$34828517376 \times 2^{2(n-12)}$

PROOF. We have exactly three separate cases for $n_1(G) = 0, 1, 2$. The proof now follows from a similar argument as the proof of Corollary 2.16 in [**9**]. $\square$

COROLLARY 3.5. *There is a connected pentacyclic graph G of order n with $n_1(G) \leqslant 2$ if and only if G belongs to one of the equivalence classes of graphs given in Tables 10, 11, 12 and 13.*

PROOF. There are three different cases for $n_1(G)$ as $n_1(G) = 0, 1, 2$. The proof now follows from an argument as the proof of Corollary 2.19 in [**9**]. $\square$

TABLE 4. Degree distributions of the connected tricyclic graphs with $n_1 = 1$ and $n_i = 0$ for $i \geqslant 8$.

E.C.	n_7	n_6	n_5	n_4	n_3	n_2	n_1	n_i	Π_2
E_1	1	0	0	0	0	$n-2$	1	0	$862683424768 \times 2^{2(n-12)}$
E_2	0	1	0	0	1	$n-3$	1	0	$330225942528 \times 2^{2(n-12)}$
E_3	0	0	1	1	0	$n-3$	1	0	$209715200000 \times 2^{2(n-12)}$
E_4	0	0	1	0	2	$n-4$	1	0	$149299200000 \times 2^{2(n-12)}$
E_5	0	0	0	2	1	$n-4$	1	0	$115964116992 \times 2^{2(n-12)}$
E_6	0	0	0	1	3	$n-5$	1	0	$82556485632 \times 2^{2(n-12)}$
E_7	0	0	0	0	5	$n-6$	1	0	$58773123072 \times 2^{2(n-12)}$

TABLE 5. Degree distributions of the connected tricyclic graphs with $n_1 = 2$ and $n_i = 0$ for $i \geqslant 9$.

E.C.	n_8	n_7	n_6	n_5	n_4	n_3	n_2	n_1	n_i	Π_2
F_1	1	0	0	0	0	0	$n-3$	2	0	$4398046511104 \times 2^{2(n-12)}$
F_2	0	1	0	0	0	1	$n-4$	2	0	$1457236279296 \times 2^{2(n-12)}$
F_3	0	0	1	0	1	0	$n-4$	2	0	$782757789696 \times 2^{2(n-12)}$
F_4	0	0	1	0	0	2	$n-5$	2	0	$557256278016 \times 2^{2(n-12)}$
F_5	0	0	0	2	0	0	$n-4$	2	0	$640000000000 \times 2^{2(n-12)}$
F_6	0	0	0	1	1	1	$n-5$	2	0	$353894400000 \times 2^{2(n-12)}$
F_7	0	0	0	1	0	3	$n-6$	2	0	$251942400000 \times 2^{2(n-12)}$
F_8	0	0	0	0	3	0	$n-5$	2	0	$274877906944 \times 2^{2(n-12)}$
F_9	0	0	0	0	2	2	$n-6$	2	0	$195689447424 \times 2^{2(n-12)}$
F_{10}	0	0	0	0	1	4	$n-7$	2	0	$139314069504 \times 2^{2(n-12)}$
F_{11}	0	0	0	0	0	6	$n-8$	2	0	$99179645184 \times 2^{2(n-12)}$

THEOREM 3.1. *Let $G_1 \in A_1$, $G_2 \in A_2$, $G_3 \in A_4$, $G_4 \in A_3$, $G_5 \in A_5$, $G_6 \in A_6$, and $G_7 \in A_8$. If G is a connected unicyclic graph with $n(\geqslant 8)$ vertices and $G \notin \{A_1, \ldots, A_6, A_8\}$, then* $\Pi_2(G_1) < \Pi_2(G_2) < \Pi_2(G_3) < \Pi_2(G_4) < \Pi_2(G_5) < \Pi_2(G_6) < \Pi_2(G_7) < \Pi_2(G)$.

PROOF. By Table 1, we have $\Pi_2(G_1) < \Pi_2(G_2) < \Pi_2(G_3) < \Pi_2(G_4) < \Pi_2(G_5) < \Pi_2(G_6) < \Pi_2(G_7)$. Now, if $n_1(G) \geqslant 5$, then Lemma 2.1, leads us to the proof. On the other hand, by the data given in Table 1, $\Pi_2(G_7) < \Pi_2(G)$, which yields the result. □

THEOREM 3.2. *Let $G_1 \in B_2$, $G_2 \in B_1$, $G_3 \in B_5$, $G_4 \in B_4$, $G_5 \in B_6$, $G_6 \in B_7$, $G_7 \in B_3$, and $G_8 \in B_{11}$. If G is a connected bicyclic graph with $n \geqslant 8$ vertices and $G \notin \{B_1, \ldots, B_7, B_{11}\}$, then* $\Pi_2(G_1) < \Pi_2(G_2) < \Pi_2(G_3) < \Pi_2(G_4) < \Pi_2(G_5) < \Pi_2(G_6) < \Pi_2(G_7) < \Pi_2(G_8) < \Pi_2(G)$.

PROOF. By Table 2, we have $\Pi_2(G_1) < \Pi_2(G_2) < \Pi_2(G_3) < \Pi_2(G_4) < \Pi_2(G_5) < \Pi_2(G_6) < \Pi_2(G_7) < \Pi_2(G_8)$. If $n_1(G) \geqslant 4$, then Lemma 2.1 leads us to the proof. On the other hand, by the data given in Table 2, $\Pi_2(G_8) < \Pi_2(G)$, which yields the result. □

TABLE 6. Degree distributions of the connected tricyclic graphs with $n_1 = 3$ and $n_i = 0$ for $i \geqslant 10$.

E.C.	n_9	n_8	n_7	n_6	n_5	n_4	n_3	n_2	n_1	n_i	Π_2
M_1	0	0	0	0	0	0	7	$n-10$	3	0	$167365651248 \times 2^{2(n-12)}$
M_2	0	0	0	0	0	1	5	$n-9$	3	0	$235092492288 \times 2^{2(n-12)}$
M_3	0	0	0	0	1	0	4	$n-8$	3	0	$425152800000 \times 2^{2(n-12)}$
M_4	0	0	0	0	0	2	3	$n-8$	3	0	$330225942528 \times 2^{2(n-14)}$
M_5	0	0	0	1	0	0	3	$n-7$	3	0	$940369969152 \times 2^{2(n-12)}$
M_6	0	0	0	0	1	1	2	$n-7$	3	0	$597196800000 \times 2^{2(n-12)}$
M_7	0	0	1	0	0	0	2	$n-6$	3	0	$2459086221312 \times 2^{2(n-12)}$
M_8	0	0	0	0	0	3	1	$n-7$	3	0	$463856467968 \times 2^{2(n-12)}$
M_9	0	0	0	1	0	1	1	$n-6$	3	0	$1320903770112 \times 2^{2(n-12)}$
M_{10}	0	0	0	0	2	0	1	$n-6$	3	0	$1080000000000 \times 2^{2(n-12)}$
M_{11}	0	1	0	0	0	0	1	$n-5$	3	0	$7421703487488 \times 2^{2(n-12)}$
M_{12}	0	0	0	0	1	2	0	$n-6$	3	0	$838860800000 \times 2^{2(n-12)}$
M_{13}	0	0	1	0	0	1	0	$n-5$	3	0	$3454189699072 \times 2^{2(n-12)}$
M_{14}	0	0	0	1	1	0	0	$n-5$	3	0	$2388787200000 \times 2^{2(n-12)}$
M_{15}	1	0	0	0	0	0	0	$n-4$	3	0	$25389989167104 \times 2^{2(n-12)}$

TABLE 7. Degree distributions of the connected tetracyclic graphs with $n_1 = 0$ and $n_i = 0$ for $i \geqslant 9$.

E.C.	n_8	n_7	n_6	n_5	n_4	n_3	n_2	n_1	n_i	Π_2
H_1	1	0	0	0	0	0	$n-1$	0	0	$70368744177664 \times 2^{2(n-12)}$
H_2	0	1	0	0	0	1	$n-2$	0	0	$23315780468736 \times 2^{2(n-12)}$
H_3	0	0	1	0	1	0	$n-2$	0	0	$12524124635136 \times 2^{2(n-12)}$
H_4	0	0	1	0	0	2	$n-3$	0	0	$8916100448256 \times 2^{2(n-12)}$
H_5	0	0	0	2	0	0	$n-2$	0	0	$10240000000000 \times 2^{2(n-12)}$
H_6	0	0	0	1	1	1	$n-3$	0	0	$5662310400000 \times 2^{2(n-12)}$
H_7	0	0	0	1	0	3	$n-4$	0	0	$4031078400000 \times 2^{2(n-12)}$
H_8	0	0	0	0	3	0	$n-3$	0	0	$4398046511104 \times 2^{2(n-12)}$
H_9	0	0	0	0	2	2	$n-4$	0	0	$3131031158784 \times 2^{2(n-12)}$
H_{10}	0	0	0	0	1	4	$n-5$	0	0	$2229025112064 \times 2^{2(n-12)}$
H_{11}	0	0	0	0	0	6	$n-6$	0	0	$1586874322944 \times 2^{2(n-12)}$

TABLE 8. Degree distributions of the connected tetracyclic graphs with $n_1 = 1$ and $n_i = 0$ for $i \geqslant 10$.

E.C.	n_9	n_8	n_7	n_6	n_5	n_4	n_3	n_2	n_1	n_i	Π_2
I_1	1	0	0	0	0	0	0	$n-2$	1	0	$406239826673664 \times 2^{2(n-12)}$
I_2	0	1	0	0	0	0	1	$n-3$	1	0	$118747255799808 \times 2^{2(n-12)}$
I_3	0	0	1	0	0	1	0	$n-3$	1	0	$55267035185152 \times 2^{2(n-12)}$
I_4	0	0	1	0	0	0	2	$n-4$	1	0	$39345379540992 \times 2^{2(n-12)}$
I_5	0	0	0	1	1	0	0	$n-3$	1	0	$38220595200000 \times 2^{2(n-12)}$
I_6	0	0	0	1	0	1	1	$n-4$	1	0	$21134460321792 \times 2^{2(n-12)}$
I_7	0	0	0	1	0	0	3	$n-5$	1	0	$15045919506432 \times 2^{2(n-12)}$
I_8	0	0	0	0	2	0	1	$n-4$	1	0	$17280000000000 \times 2^{2(n-12)}$
I_9	0	0	0	0	1	2	0	$n-4$	1	0	$13421772800000 \times 2^{2(n-12)}$
I_{10}	0	0	0	0	1	1	2	$n-5$	1	0	$9555148800000 \times 2^{2(n-12)}$
I_{11}	0	0	0	0	1	0	4	$n-6$	1	0	$6802444800000 \times 2^{2(n-12)}$
I_{12}	0	0	0	0	0	3	1	$n-5$	1	0	$7421703487488 \times 2^{2(n-12)}$
I_{13}	0	0	0	0	0	2	3	$n-6$	1	0	$5283615080448 \times 2^{2(n-12)}$
I_{14}	0	0	0	0	0	1	5	$n-7$	1	0	$3761479876608 \times 2^{2(n-12)}$
I_{15}	0	0	0	0	0	0	7	$n-8$	1	0	$2677850419968 \times 2^{2(n-12)}$

THEOREM 3.3. *Let $G_1 \in D_5$, $G_2 \in D_4$, $G_3 \in E_7$, $G_4 \in D_3$, $G_5 \in E_6$, $G_6 \in D_2$, $G_7 \in F_{11}$, $G_8 \in E_5$, $G_9 \in F_{10}$, $G_{10} \in E_4$, and $G_{11} \in M_1$. If G is a connected tricyclic graph with $n(\geqslant 10)$ vertices and $G \notin \{D_2, \ldots, D_5, E_4, \ldots, E_7, F_{10}, F_{11}, M_1\}$, then $\Pi_2(G_1) < \Pi_2(G_2) < \Pi_2(G_3) < \Pi_2(G_4) < \Pi_2(G_5) < \Pi_2(G_6) < \Pi_2(G_7) < \Pi_2(G_8) < \Pi_2(G_9) < \Pi_2(G_{10}) < \Pi_2(G_{11}) < \Pi_2(G)$.*

PROOF. By Tables 3, 4, 5, and 6 we have $\Pi_2(G_1) < \Pi_2(G_2) < \Pi_2(G_3) < \Pi_2(G_4) < \Pi_2(G_5) < \Pi_2(G_6) < \Pi_2(G_7) < \Pi_2(G_8) < \Pi_2(G_9) < \Pi_2(G_{10}) < \Pi_2(G_{11})$. Now, if $n_1(G) \geqslant 4$, then Lemma 2.1, leads us to the proof. On the other hand, by the data given in Tables 3, 4, 5, and 6, $\Pi_2(G_{11}) < \Pi_2(G)$, which yields the result. □

THEOREM 3.4. *Let $G_1 \in H_{11}$, $G_2 \in H_{10}$, $G_3 \in I_{15}$, $G_4 \in H_9$, $G_5 \in I_{14}$, $G_6 \in H_7$, $G_7 \in H_8$ and $G_8 \in N_{22}$. If G is a connected tetracyclic graph with $n \geqslant 10$ vertices and $G \notin \{H_7, \ldots, H_{11}, I_{14}, I_{15}, N_{22}\}$, then $\Pi_2(G_1) < \Pi_2(G_2) < \Pi_2(G_3) < \Pi_2(G_4) < \Pi_2(G_5) < \Pi_2(G_6) < \Pi_2(G_7) < \Pi_2(G_8) < \Pi_2(G)$.*

PROOF. By our calculation in Tables 7, 8, and 9, $\Pi_2(G_1) < \Pi_2(G_2) < \Pi_2(G_3) < \Pi_2(G_4) < \Pi_2(G_5) < \Pi_2(G_6) < \Pi_2(G_7) < \Pi_2(G_8)$. If $n_1(G) \geqslant 3$, then Lemma 2.1 gives the proof. On the other hand, by our data given in Tables 7, 8, and 9, $\Pi_2(G_8) < \Pi_2(G)$, which completes the proof. □

THEOREM 3.5. *Let $G_1 \in K_{22}$, $G_2 \in K_{21}$, $G_3 \in L_{29}$, $G_4 \in K_{20}$, $G_5 \in L_{28}$, $G_6 \in K_{17}$, $G_7 \in K_{19}$ and $G_8 \in R_{40}$. If G is a connected pentacyclic graph with $n \geqslant 12$ vertices and $G \notin \{K_{17}, K_{19}, \ldots, K_{22}, L_{28}, L_{29}, R_{40}\}$, then $\Pi_2(G_1) < \Pi_2(G_2) < \Pi_2(G_3) < \Pi_2(G_4) < \Pi_2(G_5) < \Pi_2(G_6) < \Pi_2(G_7) < \Pi_2(G_8) < \Pi_2(G)$.*

Proof. By our calculations recorded in Tables 10, 11, 12, and 13 we have $\Pi_2(G_1) < \Pi_2(G_2) < \Pi_2(G_3) < \Pi_2(G_4) < \Pi_2(G_5) < \Pi_2(G_6) < \Pi_2(G_7) < \Pi_2(G_8)$. If $n_1(G) \geqslant 3$, then Lemma 2.1 gives the proof. On the other hand, by the our data given in Tables 10, 11, 12, and 13, $\Pi_2(G_8) < \Pi_2(G)$, proving the result. □

Table 9. Degree distributions of the connected tetracyclic graphs with $n_1 = 2$ and $n_i = 0$ for $i \geqslant 11$.

E.C.	n_{10}	n_9	n_8	n_7	n_6	n_5	n_4	n_3	n_2	n_1	n_i	Π_2
N_1	1	0	0	0	0	0	0	0	$n-3$	2	0	$2621440000000000 \times 2^{2(n-12)}$
N_2	0	1	0	0	0	0	0	1	$n-4$	2	0	$685529707511808 \times 2^{2(n-12)}$
N_3	0	0	1	0	0	0	1	0	$n-4$	2	0	$281474976710656 \times 2^{2(n-12)}$
N_4	0	0	1	0	0	0	0	2	$n-5$	2	0	$200385994162176 \times 2^{2(n-12)}$
N_5	0	0	0	1	0	1	0	0	$n-4$	2	0	$168661606400000 \times 2^{2(n-12)}$
N_6	0	0	0	1	0	0	1	1	$n-5$	2	0	$93263121874944 \times 2^{2(n-12)}$
N_7	0	0	0	1	0	0	0	3	$n-6$	2	0	$66395327975424 \times 2^{2(n-12)}$
N_8	0	0	0	0	2	0	0	0	$n-4$	2	0	$142657607172096 \times 2^{2(n-12)}$
N_9	0	0	0	0	1	1	0	1	$n-5$	2	0	$64497254400000 \times 2^{2(n-12)}$
N_{10}	0	0	0	0	1	0	2	0	$n-5$	2	0	$50096498540544 \times 2^{2(n-12)}$
N_{11}	0	0	0	0	1	0	1	2	$n-6$	2	0	$35664401793024 \times 2^{2(n-12)}$
N_{12}	0	0	0	0	1	0	0	4	$n-7$	2	0	$25389989167104 \times 2^{2(n-12)}$
N_{13}	0	0	0	0	0	2	1	0	$n-5$	2	0	$40960000000000 \times 2^{2(n-12)}$
N_{14}	0	0	0	0	0	2	0	2	$n-6$	2	0	$29160000000000 \times 2^{2(n-12)}$
N_{15}	0	0	0	0	0	1	2	1	$n-6$	2	0	$22649241600000 \times 2^{2(n-12)}$
N_{16}	0	0	0	0	0	1	1	3	$n-7$	2	0	$16124313600000 \times 2^{2(n-12)}$
N_{17}	0	0	0	0	0	1	0	5	$n-8$	2	0	$11479125600000 \times 2^{2(n-12)}$
N_{18}	0	0	0	0	0	0	4	0	$n-6$	2	0	$17592186044416 \times 2^{2(n-12)}$
N_{19}	0	0	0	0	0	0	3	2	$n-7$	2	0	$12524124635136 \times 2^{2(n-12)}$
N_{20}	0	0	0	0	0	0	2	4	$n-8$	2	0	$8916100448256 \times 2^{2(n-12)}$
N_{21}	0	0	0	0	0	0	1	6	$n-9$	2	0	$6347497291776 \times 2^{2(n-12)}$
N_{22}	0	0	0	0	0	0	0	8	$n-10$	2	0	$4518872583696 \times 2^{2(n-12)}$

Theorem 3.6. *Let $G_1 \in K_{22}$. If G is a connected graph with $n(\geqslant 8)$ vertices, cyclomatic number $c(\geqslant 5)$ and $G \notin K_{22}$, then $\Pi_2(G_1) < \Pi_2(G)$.*

Proof. If $c = 5$, then Theorem 3.5 gives the proof. On the other hand, by repeated applications of Lemma 2.2, we arrive at a connected graph H, with $c = 5$ and by Lemma 2.2, $\Pi_2(H) < \Pi_2(G)$. Now, by Theorem 3.5, $\Pi_2(G_1) < \Pi_2(H) < \Pi_2(G)$, proving the result. □

Theorem 3.7. (*See* [**5**]) *Let $T_1 \in Z_1$, $T_2 \in Z_2$, $T_3 \in Z_3$, $T_4 \in Z_4$, $T_5 \in Z_5$, $T_6 \in Z_6$, $T_7 \in Z_7$ and $T_8 \in Z_8$. If T is a tree with $n(\geqslant 10)$ vertices and $T \notin \{Z_1, Z_2, \ldots, Z_8\}$, then $\Pi_2(T_1) < \Pi_2(T_2) < \Pi_2(T_3) < \Pi_2(T_4) < \Pi_2(T_5) < \Pi_2(T_6) < \Pi_2(T_7) < \Pi_2(T_8) < \Pi_2(T)$.*

We end this paper, by generalizing the main result of [**5**].

Corollary 3.6. *Let $T_1 \in Z_1$, $T_2 \in Z_2$, $T_3 \in Z_3$, $T_4 \in Z_4$, $T_5 \in Z_5$, $T_6 \in Z_6$, $T_7 \in Z_7$ and $T_8 \in Z_8$. If G is a connected graph with $n(\geqslant 10)$ vertices and $G \notin \{Z_1, Z_2, \ldots, Z_8\}$, then $\Pi_2(T_1) < \Pi_2(T_2) < \Pi_2(T_3) < \Pi_2(T_4) < \Pi_2(T_5) < \Pi_2(T_6) < \Pi_2(T_7) < \Pi_2(T_8) < \Pi_2(G)$.*

Table 10. Degree distributions of the connected pentacyclic graphs with $n_1 = 0$ and $n_i = 0$ for $i \geqslant 11$.

E.C.	n_{10}	n_9	n_8	n_7	n_6	n_5	n_4	n_3	n_2	n_1	n_i	Π_2
K_1	1	0	0	0	0	0	0	0	$n-1$	0	0	$41943040000000000 \times 2^{2(n-12)}$
K_2	0	1	0	0	0	0	0	1	$n-2$	0	0	$10968475320188928 \times 2^{2(n-12)}$
K_3	0	0	1	0	0	0	1	0	$n-2$	0	0	$4503599627370496 \times 2^{2(n-12)}$
K_4	0	0	1	0	0	0	0	2	$n-3$	0	0	$3206175906594816 \times 2^{2(n-12)}$
K_5	0	0	0	1	0	1	0	0	$n-2$	0	0	$2698585702400000 \times 2^{2(n-12)}$
K_6	0	0	0	1	0	0	1	1	$n-3$	0	0	$1492209949999104 \times 2^{2(n-12)}$
K_7	0	0	0	1	0	0	0	3	$n-4$	0	0	$1062325247606784 \times 2^{2(n-12)}$
K_8	0	0	0	0	2	0	0	0	$n-2$	0	0	$2282521714753536 \times 2^{2(n-12)}$
K_9	0	0	0	0	1	1	0	1	$n-3$	0	0	$1031956070400000 \times 2^{2(n-12)}$
K_{10}	0	0	0	0	1	0	2	0	$n-3$	0	0	$801543976648704 \times 2^{2(n-12)}$
K_{11}	0	0	0	0	1	0	1	2	$n-4$	0	0	$570630428688384 \times 2^{2(n-12)}$
K_{12}	0	0	0	0	1	0	0	4	$n-5$	0	0	$406239826673664 \times 2^{2(n-12)}$
K_{13}	0	0	0	0	0	2	1	0	$n-3$	0	0	$655360000000000 \times 2^{2(n-12)}$
K_{14}	0	0	0	0	0	2	0	2	$n-4$	0	0	$466560000000000 \times 2^{2(n-12)}$
K_{15}	0	0	0	0	0	1	2	1	$n-4$	0	0	$362387865600000 \times 2^{2(n-12)}$
K_{16}	0	0	0	0	0	1	1	3	$n-5$	0	0	$257989017600000 \times 2^{2(n-12)}$
K_{17}	0	0	0	0	0	1	0	5	$n-6$	0	0	$183666009600000 \times 2^{2(n-12)}$
K_{18}	0	0	0	0	0	0	4	0	$n-4$	0	0	$281474976710656 \times 2^{2(n-12)}$
K_{19}	0	0	0	0	0	0	3	2	$n-5$	0	0	$200385994162176 \times 2^{2(n-12)}$
K_{20}	0	0	0	0	0	0	2	4	$n-6$	0	0	$142657607172096 \times 2^{2(n-12)}$
K_{21}	0	0	0	0	0	0	1	6	$n-7$	0	0	$101559956668416 \times 2^{2(n-12)}$
K_{22}	0	0	0	0	0	0	0	8	$n-8$	0	0	$72301961339136 \times 2^{2(n-12)}$

TABLE 11. Degree distributions of the connected pentacyclic graphs with $n_1 = 1$ and $n_i = 0$ for $i \geqslant 12$.

E.C.	n_{11}	n_{10}	n_9	n_8	n_7	n_6	n_5	n_4	n_3	n_2	n_1	n_i	Π_2
L_1	1	0	0	0	0	0	0	0	0	$n-2$	1	0	$299170970322599936 \times 2^{2(n-12)}$
L_2	0	1	0	0	0	0	0	0	1	$n-3$	1	0	$70778880000000000 \times 2^{2(n-12)}$
L_3	0	0	1	0	0	0	0	1	0	$n-3$	1	0	$25999348907114496 \times 2^{2(n-12)}$
L_4	0	0	1	0	0	0	0	0	2	$n-4$	1	0	$18509302102818816 \times 2^{2(n-12)}$
L_5	0	0	0	1	0	0	1	0	0	$n-3$	1	0	$13743895347200000 \times 2^{2(n-12)}$
L_6	0	0	0	1	0	0	0	1	1	$n-4$	1	0	$7599824371187712 \times 2^{2(n-12)}$
L_7	0	0	0	1	0	0	0	0	3	$n-5$	1	0	$5410421842378752 \times 2^{2(n-12)}$
L_8	0	0	0	0	1	1	0	0	0	$n-3$	1	0	$10072417162493952 \times 2^{2(n-12)}$
L_9	0	0	0	0	1	0	1	0	1	$n-4$	1	0	$4553863372800000 \times 2^{2(n-12)}$
L_{10}	0	0	0	0	1	0	0	2	0	$n-4$	1	0	$3537090251849728 \times 2^{2(n-12)}$
L_{11}	0	0	0	0	1	0	0	1	2	$n-5$	1	0	$2518104290623488 \times 2^{2(n-12)}$
L_{12}	0	0	0	0	1	0	0	0	4	$n-6$	1	0	$1792673855336448 \times 2^{2(n-12)}$
L_{13}	0	0	0	0	0	2	0	0	1	$n-4$	1	0	$3851755393646592 \times 2^{2(n-12)}$
L_{14}	0	0	0	0	0	1	1	1	0	$n-4$	1	0	$2446118092800000 \times 2^{2(n-12)}$
L_{15}	0	0	0	0	0	1	0	2	1	$n-5$	1	0	$1352605460594688 \times 2^{2(n-12)}$
L_{16}	0	0	0	0	0	1	0	1	3	$n-6$	1	0	$962938848411648 \times 2^{2(n-12)}$
L_{17}	0	0	0	0	0	1	0	0	5	$n-7$	1	0	$685529707511808 \times 2^{2(n-12)}$
L_{18}	0	0	0	0	0	0	3	0	0	$n-4$	1	0	$2000000000000000 \times 2^{2(n-12)}$
L_{19}	0	0	0	0	0	0	2	1	1	$n-5$	1	0	$1105920000000000 \times 2^{2(n-12)}$
L_{20}	0	0	0	0	0	0	2	0	3	$n-6$	1	0	$787320000000000 \times 2^{2(n-12)}$
L_{21}	0	0	0	0	0	0	1	3	0	$n-5$	1	0	$858993459200000 \times 2^{2(n-12)}$
L_{22}	0	0	0	0	0	0	1	2	2	$n-6$	1	0	$611529523200000 \times 2^{2(n-12)}$
L_{23}	0	0	0	0	0	0	1	1	4	$n-7$	1	0	$435356467200000 \times 2^{2(n-12)}$
L_{24}	0	0	0	0	0	0	1	0	6	$n-8$	1	0	$309936391200000 \times 2^{2(n-12)}$
L_{25}	0	0	0	0	0	0	0	4	1	$n-6$	1	0	$474989023199232 \times 2^{2(n-12)}$
L_{26}	0	0	0	0	0	0	0	3	3	$n-7$	1	0	$338151365148672 \times 2^{2(n-12)}$
L_{27}	0	0	0	0	0	0	0	2	5	$n-8$	1	0	$240734712102912 \times 2^{2(n-12)}$
L_{28}	0	0	0	0	0	0	0	1	7	$n-9$	1	0	$171382426877952 \times 2^{2(n-12)}$
L_{29}	0	0	0	0	0	0	0	0	9	$n-10$	1	0	$122009559759792 \times 2^{2(n-12)}$

Table 12. Degree distributions of the connected pentacyclic graphs with $n_1 = 2$ and $n_i = 0$ for $i \geqslant 13$.

E.C.	n_{12}	n_{11}	n_{10}	n_9	n_8	n_7	n_6	n_5	n_4	n_3	n_2	n_1	n_i	Π_2
R_1	1	0	0	0	0	0	0	0	0	0	$n-3$	2	0	$2337302235907620864 \times 2^{2(n-12)}$
R_2	0	1	0	0	0	0	0	0	0	1	$n-4$	2	0	$504851012419387392 \times 2^{2(n-12)}$
R_3	0	0	1	0	0	0	0	0	1	0	$n-4$	2	0	$167772160000000000 \times 2^{2(n-12)}$
R_4	0	0	1	0	0	0	0	0	0	2	$n-5$	2	0	$119439360000000000 \times 2^{2(n-12)}$
R_5	0	0	0	1	0	0	0	1	0	0	$n-4$	2	0	$79343716147200000 \times 2^{2(n-12)}$
R_6	0	0	0	1	0	0	0	0	1	1	$n-5$	2	0	$43873901280755712 \times 2^{2(n-12)}$
R_7	0	0	0	1	0	0	0	0	0	3	$n-6$	2	0	$31234447298506752 \times 2^{2(n-12)}$
R_8	0	0	0	0	1	0	1	0	0	0	$n-4$	2	0	$51298814505517056 \times 2^{2(n-12)}$
R_9	0	0	0	0	1	0	0	1	0	1	$n-5$	2	0	$23192823398400000 \times 2^{2(n-12)}$
R_{10}	0	0	0	0	1	0	0	0	2	0	$n-5$	2	0	$18014398509481984 \times 2^{2(n-12)}$
R_{11}	0	0	0	0	1	0	0	0	1	2	$n-6$	2	0	$12824703626379264 \times 2^{2(n-12)}$
R_{12}	0	0	0	0	1	0	0	0	0	4	$n-7$	2	0	$9130086859014144 \times 2^{2(n-12)}$
R_{13}	0	0	0	0	0	2	0	0	0	0	$n-4$	2	0	$44448027302232064 \times 2^{2(n-12)}$
R_{14}	0	0	0	0	0	1	1	0	0	1	$n-5$	2	0	$16997203961708544 \times 2^{2(n-12)}$
R_{15}	0	0	0	0	0	1	0	1	1	0	$n-5$	2	0	$10794342809600000 \times 2^{2(n-12)}$
R_{16}	0	0	0	0	0	1	0	0	2	1	$n-6$	2	0	$5968839799996416 \times 2^{2(n-12)}$
R_{17}	0	0	0	0	0	1	0	0	1	3	$n-7$	2	0	$4249300990427136 \times 2^{2(n-12)}$
R_{18}	0	0	0	0	0	1	0	0	0	5	$n-8$	2	0	$3025137130880256 \times 2^{2(n-12)}$
R_{19}	0	0	0	0	0	0	2	0	1	0	$n-5$	2	0	$9130086859014144 \times 2^{2(n-12)}$
R_{20}	0	0	0	0	0	0	2	0	0	2	$n-6$	2	0	$6499837226778624 \times 2^{2(n-12)}$
R_{21}	0	0	0	0	0	0	1	2	0	0	$n-5$	2	0	$7464960000000000 \times 2^{2(n-12)}$
R_{22}	0	0	0	0	0	0	1	1	1	1	$n-6$	2	0	$4127824281600000 \times 2^{2(n-12)}$
R_{23}	0	0	0	0	0	0	1	0	3	0	$n-6$	2	0	$3206175906594816 \times 2^{2(n-12)}$
R_{24}	0	0	0	0	0	0	1	0	2	2	$n-7$	2	0	$2282521714753536 \times 2^{2(n-12)}$
R_{25}	0	0	0	0	0	0	1	0	1	4	$n-8$	2	0	$1624959306694656 \times 2^{2(n-12)}$
R_{26}	0	0	0	0	0	0	1	0	0	6	$n-9$	2	0	$1156831381426176 \times 2^{2(n-12)}$
R_{27}	0	0	0	0	0	0	0	3	0	1	$n-6$	2	0	$3375000000000000 \times 2^{2(n-12)}$
R_{28}	0	0	0	0	0	0	0	2	2	0	$n-6$	2	0	$2621440000000000 \times 2^{2(n-12)}$
R_{29}	0	0	0	0	0	0	0	2	1	2	$n-7$	2	0	$1866240000000000 \times 2^{2(n-12)}$
R_{30}	0	0	0	0	0	0	0	2	0	4	$n-8$	2	0	$1328602500000000 \times 2^{2(n-12)}$

TABLE 13. Degree distributions of the connected pentacyclic graphs with $n_1 = 2$ and $n_i = 0$ for $i \geqslant 13$.

E.C.	n_{12}	n_{11}	n_{10}	n_9	n_8	n_7	n_6	n_5	n_4	n_3	n_2	n_1	n_i	Π_2
R_{31}	0	0	0	0	0	0	0	1	3	1	$n-7$	2	0	$1449551462400000 \times 2^{2(n-12)}$
R_{32}	0	0	0	0	0	0	0	1	2	3	$n-8$	2	0	$1031956070400000 \times 2^{2(n-12)}$
R_{33}	0	0	0	0	0	0	0	1	1	5	$n-9$	2	0	$734664038400000 \times 2^{2(n-12)}$
R_{34}	0	0	0	0	0	0	0	1	0	7	$n-10$	2	0	$523017660150000 \times 2^{2(n-12)}$
R_{35}	0	0	0	0	0	0	0	0	5	0	$n-7$	2	0	$1125899906842624 \times 2^{2(n-12)}$
R_{36}	0	0	0	0	0	0	0	0	4	2	$n-8$	2	0	$801543976648704 \times 2^{2(n-12)}$
R_{37}	0	0	0	0	0	0	0	0	3	4	$n-9$	2	0	$570630428688384 \times 2^{2(n-12)}$
R_{38}	0	0	0	0	0	0	0	0	2	6	$n-10$	2	0	$406239826673664 \times 2^{2(n-12)}$
R_{39}	0	0	0	0	0	0	0	0	1	8	$n-11$	2	0	$289207845356544 \times 2^{2(n-12)}$
R_{40}	0	0	0	0	0	0	0	0	0	10	$n-12$	2	0	$205891132094649 \times 2^{2(n-12)}$

TABLE 14. Degree distributions of trees with smallest values of Π_2 with $n_i = 0$ for $i \geqslant 5$.

E.C.	n_4	n_3	n_2	n_1	n_i	Π_2
Z_1	0	0	$n-2$	2	0	$1048576 \times 2^{2(n-12)}$
Z_2	0	1	$n-4$	3	0	$1769472 \times 2^{2(n-12)}$
Z_3	0	2	$n-6$	4	0	$2985984 \times 2^{2(n-12)}$
Z_4	1	0	$n-5$	4	0	$4194304 \times 2^{2(n-12)}$
Z_5	0	3	$n-8$	5	0	$5038848 \times 2^{2(n-12)}$
Z_6	1	1	$n-7$	5	0	$7077888 \times 2^{2(n-12)}$
Z_7	0	4	$n-10$	6	0	$8503056 \times 2^{2(n-12)}$
Z_8	1	2	$n-9$	6	0	$11943936 \times 2^{2(n-12)}$

4. Concluding remarks

In this paper the extremal graphs with respect to the second multiplicative Zagreb index were determined. Our results generalize and extend the results of some earlier published papers [**18, 19, 20**]. The technique used in our considerations is efficient and can be directly applied to other degree–based topological indices.

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Receibed by editors 05.01.2018; Available online 15.01.2018.

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