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MAXIMUM SECOND ZAGREB INDEX OF TREES WITH GIVEN ROMAN DOMINATION NUMBER

AYU AMELIATUL SHAHILAH AHMAD JAMRI, ROSLAN HASNI*, MUHAMMAD KAMRAN JAMIL AND DOOST ALI MOJDEH

Abstract. Chemical study regarding total π-electron energy with respect to conjugated molecules has focused on the second Zagreb index of graphs. Moreover, in the last half-century, it has gotten a lot of attention. The relationship between the Roman domination number and the second Zagreb index is investigated in this study. We characterize the trees with the maximum second Zagreb index among those with the given Roman domination number.

1. Introduction

Chemical compounds are well-known to be expressed as graphs or chemical graphs, with vertices corresponding to atoms and edges with respect to to covalent bonds between atoms. In theoretical chemistry, predicting the physicochemical characteristics of chemical compounds is an interesting topic. Many prediction approaches for linking molecule structures with their corresponding physicochemical characteristics have been established and are still being studied. Topological indices are among the most basic of these strategies. Graph invariants are commonly termed as topological indices in chemical graph theory. Determining the extremal structures that minimize or maximize a particular topological index under specified restrictions is currently the most active topic in topological indices theory.

Assume G is a connected graph having an edge set $E(G)$ and vertex set $V(G)$. The degree of vertex u is expressed as $d(u)$. Moreover, a vertex $u \in G$ is known as pendant if $d(u) = 1$. Note that a tree comprising exactly two non-pendant vertices is known as double stars. Furthermore, the distance

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*Corresponding author.

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from u to v, expressed as $d(u,v)$, is known as the smallest length of all $u-v$ paths in G. Besides, the eccentricity of v, expressed as $ecc(v)$, stands for the maximum distance between v and other vertices in G. For other terminologies and notations not defined in this paper, the readers may refer to West [6] book.

A topological index denotes a numerical description of the molecular structure calculated from the respective molecular graph. Gutman and Trinajstić [11] established the first Zagreb index (as well as the second Zagreb index). Here, the second Zagreb index of a graph G is expressed as:

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

The second Zagreb index with several mathematical characteristics that may be found in [20, 13, 23, 21] and the comprehensive surveys [3, 10, 19, 7].

Roman dominating function (RDF) of G denotes a function $f : V(G) \to \{0,1,2\}$, which satisfies the condition such that every vertex having label 0 is adjacent to a vertex having label 2. Furthermore, the weight of an RDF f is given by $w(f) = \sum_{v \in V(G)} f(v)$. Moreover, the *Roman domination number* of G, expressed by $\gamma_R(G)$, denotes the minimum weight within all RDF in G. The Roman domination number concept of graphs was established by Cockayne *et al.* [8], which was then further investigated in [1, 12, 8, 15, 14, 4] and references therein.

For many years, scholars have been interested in the relationship between graph domination numbers and various topological indices, which has remained crucial, see [2, 18, 16, 5], the surveys of [3, 19] and references therein. In specific, Borovićanin and Furtula [2] examined the extremal Zagreb indices of trees having a specific dominance number. Furthermore, Mojdeh *et al.* [5] found some upper bounds on the Zagreb indices of trees, bicyclic as well as unicyclic graphs having a certain total domination number. When the Roman domination number is fixed, the authors in [22] determined the trees having the maximum first Zagreb index. In this paper, the trees having the maximum second Zagreb index with given Roman domination number are investigated.

2. On the maximum second Zagreb index of trees with a given Roman domination number

Let $\mathbb{T}(n, \gamma_R)$ denote the set of trees having n vertices and Roman domination number of γ_R, where $n \geq \max\left\{\lceil \frac{3\gamma_R - 5}{2} \rceil, \gamma_R + 3\right\}$.

Before analyzing the second Zagreb index of trees with given Roman domination number, it is important to recall some properties that are needed to prove our main theorems.

Lemma 2.1. [22] *Provided that T denotes a tree with a pendant vertex v. Therefore*

$$\gamma_R(T - v) \leq \gamma_R(T) \leq \gamma_R(T - v) + 1.$$

From Lemma 2.1, after deleting a pendant vertex v from a tree T, either $\gamma_R(T-v) = \gamma_R(T)$ or $\gamma_R(T-v) = \gamma_R(T) - 1$. The following lemma, present a condition in which $\gamma_R(T-v) = \gamma_R(T)$ holds.

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Lemma 2.2. [22] *Assume T is a tree. Moreover, assume that there exists (at least) three pendant vertices sharing the same neighbor in T. In particular, one of the three pendant vertices is denoted by v. Then $\gamma_R(T) = \gamma_R(T - v)$.*

The following lemma shows that the maximum degree of trees in term of Roman domination number, which is at most $n - \gamma_R(T) + 1$.

Lemma 2.3. [22] *Let $T \in \mathbb{T}(n, \gamma_R(T))$. Then $d(v) \leq n - \gamma_R(T) + 1$, for any $v \in V(T)$.*

This study focuses on the maximum degree of trees with the maximum second Zagreb index in $\mathbb{T}(n, \gamma_R)$ equals $n - \gamma_R + 1$. As a consequence, trees have a small eccentricity has been proved.

Lemma 2.4. [22] *Provided that T is a tree on n vertices having Roman domination number $\gamma_R(T)$. Here, we assume that v denotes a vertex in T having degree $n - \gamma_R(T) + 1$. Then, $ecc(v) \leq 3$.*

Before presenting the next results, we need the definition of tree branches to express the local structure of trees having the maximum second Zagreb index, see [22].

Definition 2.5. [22] *Assume T is a tree having $v \in V(T)$. We express u as the neighbor of $v \in T$. Based on T, delete all the neighbors of v except u, the component of the resulting forest containing v is known as the T branch at v.*

Besides, the authors in [22] showed exactly five possibilities for the branches at a vertex of maximum degree $n - \gamma_R(T) + 1$.

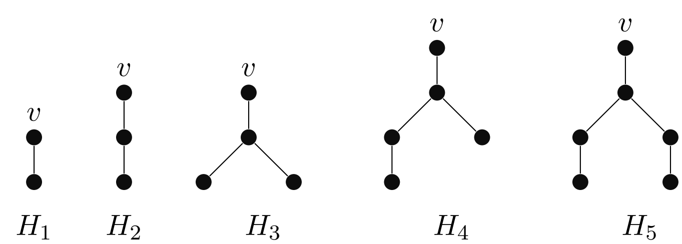

FIGURE 1. The branches occurring in Lemma 2.6.

Lemma 2.6. [22] *Assume that T denotes a tree having n vertices with Roman domination number γ_R. We let v denotes the vertex in T having degree $n - \gamma_R(T) + 1$, while H denotes the T branch at v. Thus, $H \cong H_i$, for $1 \leq i \leq 5$ (all the H_i are illustrated in Figure 1).*

Sequentially, we assume that T denotes a tree on n vertices having Roman domination number $\gamma_R(T)$. Let v be a vertex in T having degree $n - \gamma_R(T) + 1$. We also denote n_i as the number of branches H_i of T at v, for $1 \leq i \leq 5$. Then

$$n_1 + n_2 + n_3 + n_4 + n_5 = n - \gamma_R(T) + 1 \tag{2.1}$$

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and

$$n_2 + 2n_3 + 3n_4 + 4n_5 = \gamma_R(T) - 2. \tag{2.2}$$

Equation (2.1) follows from the degree $n - \gamma_R(T) + 1$ of v, and Equation (2.2) follows from the Roman domination number $\gamma_R(T)$ of T, in which the remaining vertex v are assigned as 2.

In addition, $T = (n_1, n_2, n_3, n_4, n_5)$ was used to represent a tree $T \in \mathbb{T}(n, \gamma_R)$ having n_i branches H_i of T at v, for $1 \leq i \leq 5$. When $T = (n_1, n_2, n_3, n_4, n_5)$, it is trivial to obtain

$$\begin{aligned} M_2(T) &= (n - \gamma_R(T) + 1)n_1 + (2n - 2\gamma_R(T) + 4)n_2 \\ &\quad +(3n - 3\gamma_R(T) + 9)n_3 + (3n - 3\gamma_R(T) + 14)n_4 \\ &\quad +(3n - 3\gamma_R(T) + 19)n_5. \end{aligned} \tag{2.3}$$

Proposition 2.7. *Let $T = (n_1, n_2, n_3, n_4, n_5)$ denotes a tree on n vertices having Roman domination number $\gamma_R(T)$. Therefore, each of the following conditions occur:*

(i) $n_1 \geq 1$ *and* $n_2 \geq 2$;
(ii) $n_2 \geq 2$;
(iii) $n_2 \geq 2$ *and* $n_3 \geq 1$;
(iv) $n_2 \geq 2$ *and* $n_5 \geq 1$;
(v) $n_2 \geq 2$ *and* $n_4 \geq 1$;

Proof. Set

$$T' = \begin{cases} (n_1+1, n_2-2, n_3+1, n_4, n_5) & \text{if } n_1 \geq 1 \text{ and } n_2 \geq 2 \\ (n_1+1, n_2-2, n_3+1, n_4, n_5) & \text{if } n_2 \geq 2 \\ (n_1+1, n_2-2, n_3+1, n_4, n_5) & \text{if } n_2 \geq 2 \text{ and } n_3 \geq 1 \\ (n_1+1, n_2-2, n_3+1, n_4, n_5) & \text{if } n_2 \geq 2 \text{ and } n_5 \geq 1 \\ (n_1+1, n_2-2, n_3+1, n_4, n_5) & \text{if } n_2 \geq 2 \text{ and } n_4 \geq 1 \end{cases}.$$

From Equations (2.1) and (2.2), it may be easily obtained that T' possess similar order as the Roman domination number denoted by T. Moreover, from Equation (2.3), we have that

$$M_2(T') - M_2(T) = 2.$$

It means that each of such conditions, we may construct another tree on the same order and the same Roman domination number having a larger M_2 value, which contradicts with the choosing for T (with the maximum second Zagreb index). This completes the proof. □

The equality achieved for the second Zagreb index of trees having a given Roman domination number is the subject of the following lemma.

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Proposition 2.8. *Assume that T is a tree on n vertices having Roman domination number $\gamma_R(T)$, in which $n \geq \max\left\{\lceil\frac{3\gamma_R(T)-5}{2}\rceil, \gamma_R(T)+3\right\}$. We assume that the maximum degree of T is $n-\gamma_R(T)+1$. It follows that*

$$M_2(T) \leq \begin{cases} (n-1)(n-\gamma_R(T)+1)+3\gamma_R(T)-6 & \text{if } \gamma_R(T) \text{ is even} \\ (n-1)(n-\gamma_R(T)+1)+3\gamma_R(T)-7 & \text{if } \gamma_R(T) \text{ is odd} \end{cases}.$$

In particular,

- *When $\gamma_R(T)$ is even, the equality holds if and only if* $T = \left(\frac{2n-3\gamma_R(T)+4}{2}, 0, \frac{\gamma_R(T)-2}{2}, 0, 0\right)$.
- *When $\gamma_R(T)$ is odd, the equality holds if and only if* $T = \left(\frac{2n-3\gamma_R(T)+3}{2}, 1, \frac{\gamma_R(T)-3}{2}, 0, 0\right)$ *or* $T = \left(\frac{2n-3\gamma_R(T)+5}{2}, 0, \frac{\gamma_R(T)-5}{2}, 1, 0\right)$.

Proof. Assume that $T = (n_1, n_2, n_3, n_4, n_5)$ denotes a tree having maximum second Zagreb index in $\mathbb{T}(n, \gamma_R)$. We partition the proof into two cases: $n_1 \geq 1$ and $n_1 = 0$.

Case 1. $n_1 \geq 1$.

From Proposition 2.7 (i), (v), (iv), $n_2 = 0$ or 1, $n_4 = 0$ or 1, $n_5 = 0$. Then, there exist three candidates:

(i) $n_1 = \frac{2n-3\gamma_R(T)+4}{2}$, $n_2 = 0$, $n_3 = \frac{\gamma_R(T)-2}{2}$, $n_4 = 0$, $n_5 = 0$;
(ii) $n_1 = \frac{2n-3\gamma_R(T)+3}{2}$, $n_2 = 1$, $n_3 = \frac{\gamma_R(T)-3}{2}$, $n_4 = 0$, $n_5 = 0$;
(iii) $n_1 = \frac{2n-3\gamma_R(T)+5}{2}$, $n_2 = 0$, $n_3 = \frac{\gamma_R(T)-5}{2}$, $n_4 = 1$, $n_5 = 0$.

Under the condition (i), $\gamma_R(T)$ is even, and

$$M_2(T) = (n-1)(n-\gamma_R(T)+1)+3\gamma_R(T)-6.$$

Under the conditions (ii) and (iii), in either case, $\gamma_R(T)$ is odd, and

$$M_2(T) = (n-1)(n-\gamma_R(T)+1)+3\gamma_R(T)-7.$$

Case 2. $n_1 = 0$.

Notice that $n_2 = 0$ or 1, from Proposition 2.7 (ii).

Suppose that $n_2 = 1$. Then $n_4 = n_5 = 0$ from Proposition 2.7 (iv) and (v). Furthermore, $n_3 = n - \gamma_R(T)$. It implies that $2n = 3\gamma_R(T) - 3$ with $\gamma_R(T)$ is odd, which coincides with condition (ii) mentioned above.

Next, suppose that $n_2 = 0$. Then

$$\begin{cases} n_3 + n_4 + n_5 = n - \gamma_R(T) + 1 \\ 2n_3 + 3n_4 + 4n_5 = \gamma_R(T) - 2 \end{cases}.$$

Clearly,

$$2n_3 + 3n_4 + 4n_5 \geq 2(n_3 + n_4 + n_5),$$

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equivalently $\gamma_R(T) - 2 \geq 2(n - \gamma_R(T) + 1)$, i.e., $3\gamma_R(T) - 4 \geq 2n$. Recall that $2n \geq 3\gamma_R(T) - 5$, from the hypothesis about n. So $2n = 3\gamma_R(T) - 4$ which leads to condition (i) and $2n = 3\gamma_R(T) - 5$ which leads to condition (iii).

The proof is completed now. $\square$

3. Bounds of the maximum second Zagreb index of trees with characterizations

By employing the order of trees T and the Roman domination number, we obtain an upper bound on the second Zagreb index of T, which is given in the next theorem. To simplify the calculations, we express

$$f(n, \gamma_R(T)) = \begin{cases} (n-1)(n-\gamma_R(T)+1) + 3\gamma_R(T) - 6 & \text{if } \gamma_R(T) \text{ is even} \\ (n-1)(n-\gamma_R(T)+1) + 3\gamma_R(T) - 7 & \text{if } \gamma_R(T) \text{ is odd} \end{cases}.$$

Theorem 3.1. *Assume that T is a tree on n vertices with Roman domination number $\gamma_R(T)$, where $n \geq \max\left\{\lceil \frac{3\gamma_R(T)-5}{2} \rceil, \gamma_R(T) + 3\right\}$. Then*

$$M_2(T) \leq \begin{cases} (n-1)(n-\gamma_R(T)+1) + 3\gamma_R(T) - 6 & \textit{if } \gamma_R(T) \textit{ is even} \\ (n-1)(n-\gamma_R(T)+1) + 3\gamma_R(T) - 7 & \textit{if } \gamma_R(T) \textit{ is odd} \end{cases}.$$

The equality holds for the even $\gamma_R(T)$ if and only if
$T = \left(\frac{2n-3\gamma_R(T)+4}{2}, 0, \frac{\gamma_R(T)-2}{2}, 0, 0\right)$.
For the odd $\gamma_R(T)$, the equality holds if and only if
$T = \left(\frac{2n-3\gamma_R(T)+3}{2}, 1, \frac{\gamma_R(T)-3}{2}, 0, 0\right)$ *or* $T = \left(\frac{2n-3\gamma_R(T)+5}{2}, 0, \frac{\gamma_R(T)-5}{2}, 1, 0\right)$.

Proof. Initially, we prove that $M_2(T) \leq f(n, \gamma_R(T))$, and characterize the equality cases.

From Lemma 2.3, the maximum degree of T is at most $n - \gamma_R(T) + 1$. In Proposition 2.8, we have considered the upper bound of M_2 values when the maximum degree of T is exactly $n - \gamma_R(T) + 1$. So, by using induction hypothesis, we show that $M_2(T) < f(n, \gamma_R(T))$ when the maximum degree of T is less compared to $n - \gamma_R(T) + 1$.

There is no tree whose maximum degree is less than $n - \gamma_R(T) + 1$ when $\gamma_R(T) = 2$ and 3. When $\gamma_R(T) = 4$, the trees under consideration should be double stars, the result can be checked easily. Provided that T is a tree on n vertices having Roman domination number $\gamma_R(T)$. It follows that the finding holds for every tree with order less than n as well as Roman domination number less than $\gamma_R(T)$.

From observation about a tree T: There is some vertex, say u, having $d(u) - 1$ pendant neighbors, where $d(u) \geq 2$. Let v be a pendant neighbors of u in T. Moreover, $\mu(u)$ is denoted by the sum of the vertices degrees adjacent to u.

When $d(u) \geq 4$ (u has at least three pendant neighbors), from Lemma 2.2, we get $\gamma_R(T) = \gamma_R(T-v)$. Observe that

$$\begin{aligned} & f(n, \gamma_R(T)) - f(n-1, \gamma_R(T-v)) \\ & = f(n, \gamma_R(T)) - f(n-1, \gamma_R(T)) \\ & \leq 2n - \gamma_R(T) - 1, \end{aligned}$$

and $d(u) < n - \gamma_R(T) + 1$ (this is because the maximum degree of T is less than $n - \gamma_R(T) + 1$). Thus, via the method of induction, we now have that

$$\begin{array}{rcl} M_2(T) & = & M_2(T-v) + d(u) + \mu(u) - 1 \\ & < & f(n-1, \gamma_R(T-v)) + d(u) \\ & & +[2(n-1) - d(u) - (n-1-d(u))] - 1 \\ & < & f(n-1, \gamma_R(T-v)) + (2n - \gamma_R(T) - 1) \\ & < & f(n, \gamma_R(T)), \end{array}$$

i.e., $M_2(T) < f(n, \gamma_R(T))$.

Next, assume that $d(u) = 2$ or 3 in the following. Furthermore, we assume that $\gamma_R(T-v) = \gamma_R(T) - 1$, otherwise $\gamma_R(T-v) = \gamma_R(T)$ from Lemma 2.1, which can be done by using the same method as case $d(u) \geq 4$.

For $\gamma_R(T-v) = \gamma_R(T) - 1$, it can be easily seen that

$$\begin{array}{rcl} f(n, \gamma_R(T)) - f(n-1, \gamma_R(T-v)) & = & f(n, \gamma_R(T)) - f(n-1, \gamma_R(T) - 1) \\ & = & \begin{cases} 7 & \text{if } \gamma_R(T) \text{ is even} \\ 4 & \text{if } \gamma_R(T) \text{ is odd} \end{cases}. \end{array}$$

Thus, when $d(u) = 2$, the induction hypothesis yields that

$$\begin{array}{rcl} M_2(T) & = & M_2(T-v) + 4 \\ & \leq & f(n-1, \gamma_R(T-v)) + 4 \\ & \leq & f(n, \gamma_R(T)). \end{array}$$

Notice that if $M_2(T) = f(n, \gamma_R(T))$, then $T - v$ is a tree with maximum degree $(n-1) - \gamma_R(T - v) + 1 = n - \gamma_R(T) + 1$, contradicting the hypothesis stating that T's maximum degree is less than $n - \gamma_R(T) + 1$. So $M_2(T) \leq f(n, \gamma_R(T))$.

When $d(u) = 3$, we denote v and w as the two pendant neighbours of $u \in T$. Then

$$\begin{array}{rcl} M_2(T) & = & M_2(T-v-w) + 12 \\ & \leq & f(n-2, \gamma_R(T-v-w)) + 12. \end{array}$$

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In particular, either $\gamma_R(T-v-w)=\gamma_R(T)-1$, or $\gamma_R(T-v-w)=\gamma_R(T)-2$. If $\gamma_R(T-v-w)=\gamma_R(T)-1$, then

$$\begin{aligned}&f(n,\gamma_R(T))-f(n-2,\gamma_R(T-v-w))\\&=f(n,\gamma_R(T))-f(n-2,\gamma_R(T)-1)\\&\leq 2n-2\gamma_R(T)+10\end{aligned}$$

and thus,

$$\begin{aligned}M_2(T)&\leq f(n-2,\gamma_R(T-v-w))+12\\&\leq f(n,\gamma_R(T))-(2n-2\gamma_R(T)+10)+12\\&< f(n,\gamma_R(T)),\end{aligned}$$

since $n-\gamma_R(T)+1>3$ (considering the hypothesis about the maximum degree of T). If $\gamma_R(T-v-w)=\gamma_R(T)-2$, then

$$\begin{aligned}&f(n,\gamma_R(T))-f(n-2,\gamma_R(T-v-w))\\&=f(n,\gamma_R(T))-f(n-2,\gamma_R(T)-2)\\&=12,\end{aligned}$$

and thus,

$$M_2(T)\leq f(n-2,\gamma_R(T-v-w))+12=f(n,\gamma_R(T)).$$

In particular, if $M_2(T)=f(n,\gamma_R(T))$, then $T-v-w$ is a tree with maximum degree $(n-2)-\gamma_R(T-v-w)+1=n-\gamma_R(T)+1$, which contradicts with the hypothesis that the T's maximum degree is less than $n-\gamma_R(T)+1$. So $M_2(T)\leq f(n,\gamma_R(T))$.

The proof is now completed. □

Assume we have the first three trees in the class $\mathbb{T}(n)$ with n vertices and a maximum M_2. We now let T_1, T_2 and T_3 be the trees in Figure 2. Note that the values of $\gamma_R(T_1)=2$, $\gamma_R(T_2)=3$, and $\gamma_R(T_3)=4$ are evident.

4. Concluding remarks

This paper is devoted to the investigation of relationship between the second Zagreb index and Roman domination number of trees. More precisely, we provide an upper bound for the second Zagreb index of trees with regards to the Roman domination number, where we describe those tree(s) that achieve equality.

As a possible sequel in the future, it is interesting to investigate the relationship between the second Zagreb index (or other well-known topological indices, e.g., Randić index, Wiener index) and other types of domination number of graphs.

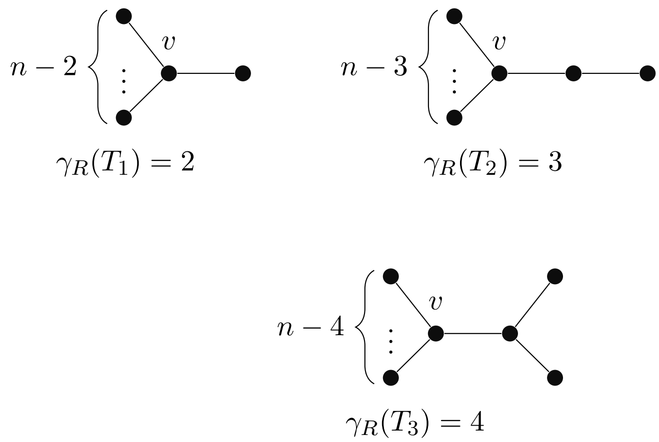

FIGURE 2. The three extremal trees of second Zagreb Index.

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Ayu Ameliatul Shahilah Ahmad Jamri

Special Interest Group on Modelling and Data Analytics (SIGMDA), Faculty of Ocean Engineering Technology and Informatics, Universiti Malaysia Terengganu, 21030 Kuala Nerus, Terengganu, Malaysia

Email: ayu_amyliatul@yahoo.com

Roslan Hasni

Special Interest Group on Modelling and Data Analytics (SIGMDA), Faculty of Ocean Engineering Technology and Informatics, Universiti Malaysia Terengganu, 21030 Kuala Nerus, Terengganu, Malaysia

Email: hroslan@umt.edu.my

Muhammad Kamran Jamil

Department of Mathematics, Riphah International University, Lahore, Pakistan

Email: m.kamran.sms@gmail.com

Doost Ali Mojdeh

Department of Mathematics, University of Mazandran, Babolsar, Iran

Email: damojdeh@umz.ac.ir