

Some Results on Vertex Version and Edge Versions of Modified Schultz Index

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Abstract: Let G_1 and G_2 be two simple connected graphs with disjoint vertex sets $V(G_1)$ and $V(G_2)$, respectively. For given vertices $a_1 \in V(G_1)$ and $a_2 \in V(G_2)$, a splice of G_1 and G_2 by vertices a_1 and a_2 is defined by identifying the vertices a_1 and a_2 in the union of G_1 and G_2 and a link of G_1 and G_2 by vertices a_1 and a_2 is obtained by joining a_1 and a_2 by an edge in the union of these graphs. The modified Schultz index of a simple connected graph G is defined as the sum of the terms $d(u|G)d(v|G)d(u, v|G)$ over all unordered pairs $\{u, v\}$ of vertices in G , where $d(u|G)$ and $d(u, v|G)$ denote the degree of the vertex u of G and the distance between the vertices u and v of G , respectively. In this paper, explicit formulas for computing the vertex and edge-modified Schultz indices of splice and link of graphs are presented.

Key Words: Distance, vertex-degree, modified Schultz index, edge-modified Schultz index, splice, link.

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§1. Introduction

In this paper, we consider connected finite graphs without any loops or multiple edges. A *topological index* $Top(G)$ of a graph G is a real number with the property that for every graph H isomorphic to G , $Top(H) = Top(G)$. There are numerous topological indices that have been found to be useful in chemical documentation, isomer discrimination, quantitative structure-property relationships (QSPR), quantitative structure-activity relationships (QSAR), and pharmaceutical drug design [7, 10]. The *Wiener index* is the first reported distance-based topological index which was introduced in 1947 by Wiener [19, 20] 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 ,

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

where $d(u, v | G)$ denotes the distance between the vertices u and v of G which is defined as the

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length of any shortest path in G connecting them.

The *molecular topological index* or *Schultz index* [17] was introduced by Harry Schultz in 1989. The Schultz index of a graph G is defined as

$$S(G) = \sum_{\{u,v\} \subseteq V(G)} [d(u|G) + d(v|G)]d(u,v|G),$$

where $d(u|G)$ denotes the degree of the vertex u of G .

The vertex version of the *modified Schultz index* [9] of a graph G was introduced by Ivan Gutman in 1994 as

$$S^*(G) = \sum_{\{u,v\} \subseteq V(G)} d(u|G)d(v|G)d(u,v|G).$$

The modified Schultz index is also known as *Gutman index*.

The edge versions of the modified Schultz index [15] were introduced by Khormali *et al.* in 2010. Two possible distances between the edges $e = uv$ and $f = zt$ of a graph G can be considered. The first distance is denoted by $d_0(e, f|G)$ and defined as

$$d_0(e, f|G) = \begin{cases} d_1(e, f|G) + 1 & e \neq f, \\ 0 & e = f, \end{cases}$$

where $d_1(e, f|G) = \min\{d(u, z|G), d(u, t|G), d(v, z|G), d(v, t|G)\}$. It is easy to see that, $d_0(e, f|G) = d(e, f|L(G))$, where $L(G)$ is the line graph of G .

The second distance is denoted by $d_4(e, f|G)$ and defined as

$$d_4(e, f|G) = \begin{cases} d_2(e, f|G) & e \neq f, \\ 0 & e = f, \end{cases}$$

where $d_2(e, f|G) = \max\{d(u, z|G), d(u, t|G), d(v, z|G), d(v, t|G)\}$.

Related to the distances d_0 and d_4 , two edge versions of the modified Schultz index can be defined. The first and second *edge-modified Schultz indices* of G are denoted by $(W_*)_{e_0}(G)$ and $(W_*)_{e_4}(G)$, respectively and defined as

$$(W_*)_{e_i}(G) = \sum_{\{e,f\} \subseteq E(G)} d(e|G)d(f|G)d_i(e, f|G), \quad i \in \{0, 4\},$$

where $d(e|G)$ denotes the degree of the edge e in G which is the degree of the vertex e in the line graph $L(G)$. For more information on the edge-modified Schultz indices, see [14].

In this paper, we compute the vertex version and edge versions of the modified-Schultz index for splice and link of graphs. Readers interested in more information on computing topological indices of splice and link of graphs can be referred to [1 C 6, 8, 12, 13, 16, 18].

§2. Definitions and Preliminaries

Let G be a graph with vertex set $V(G)$ and edge set $E(G)$. We denote by $V(e)$ the set of two

end-vertices of the edge e of G . For $u \in V(G)$ and $e = ab \in E(G)$, we define

$$D_1(u, e | G) = \min\{d(u, a | G), d(u, b | G)\}, \quad D_2(u, e | G) = \max\{d(u, a | G), d(u, b | G)\}.$$

Note that, $D_1(u, e | G)$ is a nonnegative integer and $D_1(u, e | G) = 0$ if and only if $u \in V(e)$. Also, $D_2(u, e | G)$ is a positive integer and $D_2(u, e | G) = 1$ if and only if $u \in V(e)$ or u and the end vertices of e form a 3-cycle in G .

For $u \in V(G)$, let $N(u | G)$ denote the set of all first neighbors of u in G . We denote by $\delta(u | G)$, the sum of degrees of all neighbors of u in G , i.e.,

$$\delta(u | G) = \sum_{v \in N(u | G)} d(v | G).$$

We denote by $M_1(G)$, the *first Zagreb index* [11] of G which is defined as

$$M_1(G) = \sum_{u \in V(G)} d(u | G)^2.$$

The first Zagreb index can also be expressed as a sum over edges of G ,

$$M_1(G) = \sum_{uv \in E(G)} [d(u | G) + d(v | G)].$$

Let e be an edge of G with $V(e) = \{a, b\}$. It is easy to see that, $d(e | G) = d(a | G) + d(b | G) - 2$. Therefore,

$$\sum_{e \in E(G)} d(e | G) = M_1(G) - 2|E(G)|.$$

Also for $u \in V(G)$, we have

$$\sum_{e \in E(G); u \in V(e)} d(e | G) = d(u | G)(d(u | G) - 2) + \delta(u | G),$$

$$\sum_{\{e, f\} \subseteq E(G); u \in V(e) \cap V(f)} [d(e | G) + d(f | G)] = (d(u | G) - 1)[d(u | G)(d(u | G) - 2) + \delta(u | G)].$$

§3. Results and Discussion

In this section, we compute the vertex version and edge versions of the modified Schultz index for splice and link of graphs.

3.1 Splice

Let G_1 and G_2 be two graphs with disjoint vertex sets $V(G_1)$ and $V(G_2)$ and edge sets $E(G_1)$ and $E(G_2)$, respectively. For given vertices $a_1 \in V(G_1)$ and $a_2 \in V(G_2)$, a *splice* [8] of G_1 and G_2 by vertices a_1 and a_2 is denoted by $(G_1.G_2)(a_1, a_2)$ and defined by identifying the vertices

a_1 and a_2 in the union of G_1 and G_2 . We denote by n_i , m_i and α_i , the order and size of the graph G_i and the degree of a_i in G_i , respectively, where $i \in \{1, 2\}$. It is easy to see that, $|V((G_1.G_2)(a_1, a_2))| = n_1 + n_2 - 1$ and $|E((G_1.G_2)(a_1, a_2))| = m_1 + m_2$.

In the following lemmas, the degree of an arbitrary vertex of $(G_1.G_2)(a_1, a_2)$ and the distance between two arbitrary vertices of this graph are computed. The results follow easily from the definition of the splice of graphs, so their proofs are omitted.

Lemma 3.1 *Let $u \in V((G_1.G_2)(a_1, a_2))$. Then*

$$d(u | (G_1.G_2)(a_1, a_2)) = \begin{cases} d(u | G_1) & u \in V(G_1) \setminus \{a_1\}, \\ d(u | G_2) & u \in V(G_2) \setminus \{a_2\}, \\ \alpha_1 + \alpha_2 & u = a_1 \text{ or } u = a_2. \end{cases}$$

Lemma 3.2 *Let $u, v \in V((G_1.G_2)(a_1, a_2))$. Then*

$$d(u, v | (G_1.G_2)(a_1, a_2)) = \begin{cases} d(u, v | G_1) & u, v \in V(G_1), \\ d(u, v | G_2) & u, v \in V(G_2), \\ d(u, a_1 | G_1) + d(a_2, v | G_2) & u \in V(G_1), v \in V(G_2). \end{cases}$$

In the following theorem, the modified Schultz index of $(G_1.G_2)(a_1, a_2)$ is computed.

Theorem 3.3 *The modified Schultz index of $G = (G_1.G_2)(a_1, a_2)$ is given by*

$$\begin{aligned} S^*(G) = & S^*(G_1) + S^*(G_2) + 2m_2 \sum_{u \in V(G_1) \setminus \{a_1\}} d(u | G_1) d(u, a_1 | G_1) \\ & + 2m_1 \sum_{u \in V(G_2) \setminus \{a_2\}} d(u | G_2) d(u, a_2 | G_2). \end{aligned}$$

Proof We partition the sum in the formula of $S^*(G)$ into three sums as follows.

The first sum S_1 consists of contributions to $S^*(G)$ of pairs of vertices from G_1 . Using Lemmas 3.1 and 3.2, we obtain

$$\begin{aligned} S_1 = & \sum_{\{u, v\} \subseteq V(G_1) \setminus \{a_1\}} d(u | G_1) d(v | G_1) d(u, v | G_1) \\ & + (\alpha_1 + \alpha_2) \sum_{u \in V(G_1) \setminus \{a_1\}} d(u | G_1) d(u, a_1 | G_1) \\ = & S^*(G_1) + \alpha_2 \sum_{u \in V(G_1) \setminus \{a_1\}} d(u | G_1) d(u, a_1 | G_1). \end{aligned}$$

The second sum S_2 consists of contributions to $S^*(G)$ of pairs of vertices from G_2 . Similar

to the previous case, we obtain

$$S_2 = S^*(G_2) + \alpha_1 \sum_{u \in V(G_2) \setminus \{a_2\}} d(u|G_2)d(u, a_2|G_2).$$

The third sum S_3 is taken over all pairs $\{u, v\}$ of vertices in G such that $u \in V(G_1) \setminus \{a_1\}$ and $v \in V(G_2) \setminus \{a_2\}$. Using Lemmas 3.1 and 3.2, we obtain

$$\begin{aligned} S_3 &= \sum_{u \in V(G_1) \setminus \{a_1\}} \sum_{v \in V(G_2) \setminus \{a_2\}} d(u|G_1)d(v|G_2)[d(u, a_1|G_1) + d(a_2, v|G_2)] \\ &= (2m_2 - \alpha_2) \sum_{u \in V(G_1) \setminus \{a_1\}} d(u|G_1)d(u, a_1|G_1) \\ &\quad + (2m_1 - \alpha_1) \sum_{u \in V(G_2) \setminus \{a_2\}} d(u|G_2)d(u, a_2|G_2). \end{aligned}$$

The formula of $S^*(G)$ is obtained by adding S_1 , S_2 and S_3 and simplifying the resulting expression. \square

In the following lemmas, the degree of an arbitrary edge of $(G_1.G_2)(a_1, a_2)$ and the distances d_0 and d_4 between two arbitrary edges of this graph are computed. The results are direct consequences of Lemmas 3.1 and 3.2, respectively, so their proofs are omitted.

Lemma 3.4 *Let $e \in E((G_1.G_2)(a_1, a_2))$. Then*

$$d(e|(G_1.G_2)(a_1, a_2)) = \begin{cases} d(e|G_1) & e \in E(G_1), a_1 \notin V(e), \\ d(e|G_1) + \alpha_2 & e \in E(G_1), a_1 \in V(e), \\ d(e|G_2) & e \in E(G_2), a_2 \notin V(e), \\ d(e|G_2) + \alpha_1 & e \in E(G_2), a_2 \in V(e). \end{cases}$$

Lemma 3.5 *Let $G = (G_1.G_2)(a_1, a_2)$ and $e, f \in E(G)$. Then*

$$(i) \quad d_0(e, f|G) = \begin{cases} d_0(e, f|G_1) & e, f \in E(G_1), \\ d_0(e, f|G_2) & e, f \in E(G_2), \\ D_1(a_1, e|G_1) + D_1(a_2, f|G_2) + 1 & e \in E(G_1), f \in E(G_2), \end{cases}$$

$$(ii) \quad d_4(e, f|G) = \begin{cases} d_4(e, f|G_1) & e, f \in E(G_1), \\ d_4(e, f|G_2) & e, f \in E(G_2), \\ D_2(a_1, e|G_1) + D_2(a_2, f|G_2) & e \in E(G_1), f \in E(G_2). \end{cases}$$

In the following theorem, the first and second edge-modified Schultz indices of $(G_1.G_2)(a_1, a_2)$ are computed.

Theorem 3.6 *The first and second edge-modified Schultz indices of $G = (G_1.G_2)(a_1, a_2)$ are*

given by

$$\begin{aligned}
(i) \quad (W_*)_{e_0}(G) &= (W_*)_{e_0}(G_1) + (W_*)_{e_0}(G_2) \\
&+ \alpha_2 \sum_{e,f \in E(G_1); a_1 \in V(e) \setminus V(f)} d(f|G_1) d_0(e, f|G_1) \\
&+ \alpha_1 \sum_{e,f \in E(G_2); a_2 \in V(e) \setminus V(f)} d(f|G_2) d_0(e, f|G_2) \\
&+ (M_1(G_2) - 2m_2 + \alpha_1\alpha_2) \sum_{e \in E(G_1)} d(e|G_1) D_1(a_1, e|G_1) \\
&+ (M_1(G_1) - 2m_1 + \alpha_1\alpha_2) \sum_{f \in E(G_2)} d(f|G_2) D_1(a_2, f|G_2) \\
&+ (M_1(G_1) - 2m_1)(M_1(G_2) - 2m_2) + \alpha_2(\alpha_1 - 1)\delta(a_1|G_1) + \alpha_1(\alpha_2 - 1)\delta(a_2|G_2) \\
&+ \alpha_1\alpha_2 [M_1(G_1) + M_1(G_2) + (\alpha_1 + \alpha_2)^2 - \frac{7}{2}(\alpha_1 + \alpha_2) - 2(m_1 + m_2 - 2)]. \\
(ii) \quad (W_*)_{e_4}(G) &= (W_*)_{e_4}(G_1) + (W_*)_{e_4}(G_2) \\
&+ \alpha_2 \sum_{e,f \in E(G_1); a_1 \in V(e) \setminus V(f)} d(f|G_1) d_4(e, f|G_1) \\
&+ \alpha_1 \sum_{e,f \in E(G_2); a_2 \in V(e) \setminus V(f)} d(f|G_2) d_4(e, f|G_2) \\
&+ (M_1(G_2) - 2m_2 + \alpha_1\alpha_2) \sum_{e \in E(G_1)} d(e|G_1) D_2(a_1, e|G_1) \\
&+ (M_1(G_1) - 2m_1 + \alpha_1\alpha_2) \sum_{f \in E(G_2)} d(f|G_2) D_2(a_2, f|G_2) \\
&+ \alpha_2 \sum_{\{u,v\} \subseteq N(a_1|G_1)} [d(u|G_1) + d(v|G_1)] d(u, v|G_1) \\
&+ \alpha_1 \sum_{\{u,v\} \subseteq N(a_2|G_2)} [d(u|G_2) + d(v|G_2)] d(u, v|G_2) \\
&+ \alpha_2(\alpha_2 + 2\alpha_1 - 4) \sum_{\{u,v\} \subseteq N(a_1|G_1)} d(u, v|G_1) \\
&+ \alpha_1(\alpha_1 + 2\alpha_2 - 4) \sum_{\{u,v\} \subseteq N(a_2|G_2)} d(u, v|G_2) \\
&+ \alpha_1\alpha_2 [M_1(G_1) + M_1(G_2) - 2(m_1 + m_2 - \alpha_1\alpha_2)].
\end{aligned}$$

Proof We prove the first part of the theorem. The second part can be proved by a similar method. At first, we partition the sum in the formula of $(W_*)_{e_0}(G)$ into three sums as follows.

The first sum S_1 consists of contributions to $(W_*)_{e_0}(G)$ of pairs of edges from G_1 . In order to compute S_1 , we partition it into three sums S_{11} , S_{12} and S_{13} as follows.

The sum S_{11} is equal to

$$S_{11} = \sum_{\{e,f\} \subseteq E(G_1); a_1 \notin V(e) \cup V(f)} d(e|G) d(f|G) d_0(e, f|G).$$

Using Lemmas 3.4 and 3.5, we obtain

$$S_{11} = \sum_{\{e,f\} \subseteq E(G_1); a_1 \notin V(e) \cup V(f)} d(e|G_1)d(f|G_1)d_0(e,f|G_1).$$

The sum S_{12} is equal to

$$S_{12} = \sum_{\{e,f\} \subseteq E(G_1); a_1 \in V(e) \cap V(f)} d(e|G)d(f|G)d_0(e,f|G).$$

Note that, for every pairs $\{e, f\}$ of edges in G_1 such that $a_1 \in V(e) \cap V(f)$, $d_0(e, f|G_1) = 1$. Now, using Lemmas 3.4 and 3.5, we obtain

$$\begin{aligned} S_{12} &= \sum_{\{e,f\} \subseteq E(G_1); a_1 \in V(e) \cap V(f)} (d(e|G_1) + \alpha_2)(d(f|G_1) + \alpha_2) \\ &= \sum_{\{e,f\} \subseteq E(G_1); a_1 \in V(e) \cap V(f)} d(e|G_1)d(f|G_1) \\ &\quad + \alpha_2(\alpha_1 - 1)[\alpha_1(\alpha_1 - 2) + \delta(a_1|G_1)] + \alpha_2^2 \binom{\alpha_1}{2}. \end{aligned}$$

The sum S_{13} is equal to

$$S_{13} = \sum_{e,f \in E(G_1); a_1 \in V(e) \setminus V(f)} d(e|G)d(f|G)d_0(e,f|G).$$

Using Lemmas 3.4 and 3.5, we obtain

$$\begin{aligned} S_{13} &= \sum_{e,f \in E(G_1); a_1 \in V(e) \setminus V(f)} (d(e|G_1) + \alpha_2)d(f|G_1)d_0(e,f|G_1) \\ &= \sum_{e,f \in E(G_1); a_1 \in V(e) \setminus V(f)} d(e|G_1)d(f|G_1)d_0(e,f|G_1) \\ &\quad + \alpha_2 \sum_{e,f \in E(G_1); a_1 \in V(e) \setminus V(f)} d(f|G_1)d_0(e,f|G_1). \end{aligned}$$

By adding S_{11} , S_{12} and S_{13} , we obtain

$$\begin{aligned} S_1 &= (W_*)_{e_0}(G_1) + \alpha_2^2 \binom{\alpha_1}{2} + \alpha_2(\alpha_1 - 1)[\alpha_1(\alpha_1 - 2) + \delta(a_1|G_1)] \\ &\quad + \alpha_2 \sum_{e,f \in E(G_1); a_1 \in V(e) \setminus V(f)} d(f|G_1)d_0(e,f|G_1). \end{aligned}$$

The second sum S_2 consists of contributions to $(W_*)_{e_0}(G)$ of pairs of edges from G_2 .

Using the same argument as in the computation of S_1 , we obtain

$$S_2 = (W_*)_{e_0}(G_2) + \alpha_1^2 \binom{\alpha_2}{2} + \alpha_1(\alpha_2 - 1)[\alpha_2(\alpha_2 - 2) + \delta(a_2 | G_2)] \\ + \alpha_1 \sum_{e, f \in E(G_2); a_2 \in V(e) \setminus V(f)} d(f | G_2) d_0(e, f | G_2).$$

The third sum S_3 is taken over all pairs $\{e, f\}$ of edges in G such that $e \in E(G_1)$ and $f \in E(G_2)$. In order to compute S_3 , we partition it into four sums S_{31} , S_{32} , S_{33} and S_{34} as follows.

The sum S_{31} is equal to

$$S_{31} = \sum_{e \in E(G_1); a_1 \notin V(e)} \sum_{f \in E(G_2); a_2 \notin V(f)} d(e | G) d(f | G) d_0(e, f | G).$$

Using Lemmas 3.4 and 3.5, we obtain

$$S_{31} = \sum_{e \in E(G_1); a_1 \notin V(e)} \sum_{f \in E(G_2); a_2 \notin V(f)} d(e | G_1) d(f | G_2) [D_1(a_1, e | G_1) + D_1(a_2, f | G_2) + 1] \\ = [M_1(G_2) - 2m_2 - \alpha_2(\alpha_2 - 2) - \delta(a_2 | G_2)] \sum_{e \in E(G_1)} d(e | G_1) D_1(a_1, e | G_1) \\ + [M_1(G_1) - 2m_1 - \alpha_1(\alpha_1 - 2) - \delta(a_1 | G_1)] \sum_{f \in E(G_2)} d(f | G_2) D_1(a_2, f | G_2) \\ + [M_1(G_1) - 2m_1 - \alpha_1(\alpha_1 - 2) - \delta(a_1 | G_1)] \\ \times [M_1(G_2) - 2m_2 - \alpha_2(\alpha_2 - 2) - \delta(a_2 | G_2)].$$

The sum S_{32} is equal to

$$S_{32} = \sum_{e \in E(G_1); a_1 \notin V(e)} \sum_{f \in E(G_2); a_2 \in V(f)} d(e | G) d(f | G) d_0(e, f | G).$$

Using Lemmas 3.4 and 3.5, we obtain

$$S_{32} = \sum_{e \in E(G_1); a_1 \notin V(e)} \sum_{f \in E(G_2); a_2 \in V(f)} d(e | G_1) (d(f | G_2) + \alpha_1) [D_1(a_1, e | G_1) + 1] \\ = [\alpha_2(\alpha_2 - 2) + \delta(a_2 | G_2) + \alpha_1 \alpha_2] \left[\sum_{e \in E(G_1)} d(e | G_1) D_1(a_1, e | G_1) \right. \\ \left. + M_1(G_1) - 2m_1 - \alpha_1(\alpha_1 - 2) - \delta(a_1 | G_1) \right].$$

The sum S_{33} is equal to

$$S_{33} = \sum_{e \in E(G_1); a_1 \in V(e)} \sum_{f \in E(G_2); a_2 \notin V(f)} d(e | G) d(f | G) d_0(e, f | G).$$

Using the same argument as in the computation of S_{32} , we obtain

$$S_{33} = [\alpha_1(\alpha_1 - 2) + \delta(a_1 | G_1) + \alpha_1\alpha_2] \left[\sum_{f \in E(G_2)} d(f | G_2) D_1(a_2, f | G_2) \right. \\ \left. + M_1(G_2) - 2m_2 - \alpha_2(\alpha_2 - 2) - \delta(a_2 | G_2) \right].$$

The sum S_{34} is equal to

$$S_{34} = \sum_{e \in E(G_1); a_1 \in V(e)} \sum_{f \in E(G_2); a_2 \in V(f)} d(e | G) d(f | G) d_0(e, f | G).$$

Using Lemmas 3.4 and 3.5, we obtain

$$S_{34} = \sum_{e \in E(G_1); a_1 \in V(e)} \sum_{f \in E(G_2); a_2 \in V(f)} (d(e | G_1) + \alpha_2)(d(f | G_2) + \alpha_1) \\ = [\alpha_1(\alpha_1 - 2) + \delta(a_1 | G_1) + \alpha_1\alpha_2] [\alpha_2(\alpha_2 - 2) + \delta(a_2 | G_2) + \alpha_1\alpha_2].$$

By adding S_{31} , S_{32} , S_{33} and S_{34} , we obtain

$$S_3 = (M_1(G_2) - 2m_2 + \alpha_1\alpha_2) \sum_{e \in E(G_1)} d(e | G_1) D_1(a_1, e | G_1) \\ + (M_1(G_1) - 2m_1 + \alpha_1\alpha_2) \sum_{f \in E(G_2)} d(f | G_2) D_1(a_2, f | G_2) \\ + (M_1(G_1) - 2m_1)(M_1(G_2) - 2m_2) \\ + \alpha_1\alpha_2 [M_1(G_1) - 2m_1 + M_1(G_2) - 2m_2 + \alpha_1\alpha_2].$$

The formula of $(W_*)_{e_0}(G)$ is obtained by adding S_1 , S_2 and S_3 and simplifying the resulting expression. \square

3.2 Link

Let G_1 and G_2 be two graphs with disjoint vertex sets $V(G_1)$ and $V(G_2)$ and edge sets $E(G_1)$ and $E(G_2)$, respectively. For vertices $a_1 \in V(G_1)$ and $a_2 \in V(G_2)$, a *link* [8] of G_1 and G_2 by vertices a_1 and a_2 is denoted by $(G_1 \sim G_2)(a_1, a_2)$ and obtained by joining a_1 and a_2 by an edge in the union of these graphs. We denote by n_i , m_i and α_i , the order and size of the graph G_i and the degree of a_i in G_i , respectively, where $i \in \{1, 2\}$. It is easy to see that, $|V((G_1 \sim G_2)(a_1, a_2))| = n_1 + n_2$ and $|E((G_1 \sim G_2)(a_1, a_2))| = m_1 + m_2 + 1$.

In the following lemmas, the degree of an arbitrary vertex of $(G_1 \sim G_2)(a_1, a_2)$ and the distance between two arbitrary vertices of this graph are computed. The results follow easily from the definition of the link of graphs, so their proofs are omitted.

Lemma 3.7 *Let $u \in V((G_1 \sim G_2)(a_1, a_2))$. Then*

$$d(u | (G_1 \sim G_2)(a_1, a_2)) = \begin{cases} d(u | G_1) & u \in V(G_1) \setminus \{a_1\}, \\ d(u | G_2) & u \in V(G_2) \setminus \{a_2\}, \\ \alpha_1 + 1 & u = a_1, \\ \alpha_2 + 1 & u = a_2. \end{cases}$$

Lemma 3.8 *Let $u, v \in V((G_1 \sim G_2)(a_1, a_2))$. Then*

$$d(u, v | (G_1 \sim G_2)(a_1, a_2)) = \begin{cases} d(u, v | G_1) & u, v \in V(G_1), \\ d(u, v | G_2) & u, v \in V(G_2), \\ d(u, a_1 | G_1) + d(a_2, v | G_2) + 1 & u \in V(G_1), v \in V(G_2). \end{cases}$$

In the following theorem, the modified Schultz index of $(G_1 \sim G_2)(a_1, a_2)$ is computed.

Theorem 3.9 *The modified Schultz index of $G = (G_1 \sim G_2)(a_1, a_2)$ is given by*

$$\begin{aligned} S^*(G) = & S^*(G_1) + S^*(G_2) + 2(m_2 + 1) \sum_{u \in V(G_1) \setminus \{a_1\}} d(u | G_1) d(u, a_1 | G_1) \\ & + 2(m_1 + 1) \sum_{u \in V(G_2) \setminus \{a_2\}} d(u | G_2) d(u, a_2 | G_2) + 2(m_1 + m_2 + 2m_1 m_2) + 1. \end{aligned}$$

Proof We partition the sum in the formula of $S^*(G)$ into three sums as follows.

The first sum S_1 consists of contributions to $S^*(G)$ of pairs of vertices from G_1 . By Lemmas 3.7 and 3.8, we obtain

$$\begin{aligned} S_1 = & \sum_{\{u, v\} \subseteq V(G_1) \setminus \{a_1\}} d(u | G_1) d(v | G_1) d(u, v | G_1) \\ & + (\alpha_1 + 1) \sum_{u \in V(G_1) \setminus \{a_1\}} d(u | G_1) d(u, a_1 | G_1) \\ = & S^*(G_1) + \sum_{u \in V(G_1) \setminus \{a_1\}} d(u | G_1) d(u, a_1 | G_1). \end{aligned}$$

The second sum S_2 consists of contributions to $S^*(G)$ of pairs of vertices from G_2 . Similar to the previous case, we obtain

$$S_2 = S^*(G_2) + \sum_{u \in V(G_2) \setminus \{a_2\}} d(u | G_2) d(u, a_2 | G_2).$$

The third sum S_3 is taken over all pairs $\{u, v\}$ of vertices in G such that $u \in V(G_1)$ and $v \in V(G_2)$. In order to compute S_3 , we partition it into four sums S_{31} , S_{32} , S_{33} and S_{34} as

follows.

The sum S_{31} is taken over all pairs $\{u, v\}$ of vertices in G such that $u \in V(G_1) \setminus \{a_1\}$ and $v = a_2$. Using Lemmas 3.7 and 3.8, we obtain

$$\begin{aligned} S_{31} &= (\alpha_2 + 1) \sum_{u \in V(G_1) \setminus \{a_1\}} d(u | G_1) [d(u, a_1 | G_1) + 1] \\ &= (\alpha_2 + 1) \left[\sum_{u \in V(G_1) \setminus \{a_1\}} d(u | G_1) d(u, a_1 | G_1) + 2m_1 - \alpha_1 \right]. \end{aligned}$$

The sum S_{32} is taken over all pairs $\{u, v\}$ of vertices in G such that $u \in V(G_2) \setminus \{a_2\}$ and $v = a_1$. Similar to the previous case, we obtain

$$S_{32} = (\alpha_1 + 1) \left[\sum_{u \in V(G_2) \setminus \{a_2\}} d(u | G_2) d(u, a_2 | G_2) + 2m_2 - \alpha_2 \right].$$

The sum S_{33} is taken over all pairs $\{u, v\}$ of vertices in G such that $u \in V(G_1) \setminus \{a_1\}$ and $v \in V(G_2) \setminus \{a_2\}$. By Lemmas 3.7 and 3.8, we obtain

$$\begin{aligned} S_{33} &= \sum_{u \in V(G_1) \setminus \{a_1\}} \sum_{v \in V(G_2) \setminus \{a_2\}} d(u | G_1) d(v | G_2) [d(u, a_1 | G_1) + d(a_2, v | G_2) + 1] \\ &= (2m_2 - \alpha_2) \sum_{u \in V(G_1) \setminus \{a_1\}} d(u | G_1) d(u, a_1 | G_1) \\ &\quad + (2m_1 - \alpha_1) \sum_{v \in V(G_2) \setminus \{a_2\}} d(v | G_2) d(a_2, v | G_2) + (2m_1 - \alpha_1)(2m_2 - \alpha_2). \end{aligned}$$

The sum S_{34} is equal to

$$S_{34} = d(a_1 | G) d(a_2 | G) d(a_1, a_2 | G) = (\alpha_1 + 1)(\alpha_2 + 1).$$

By adding S_{31} , S_{32} , S_{33} and S_{34} , we obtain

$$\begin{aligned} S_3 &= (2m_2 + 1) \sum_{u \in V(G_1) \setminus \{a_1\}} d(u | G_1) d(u, a_1 | G_1) \\ &\quad + (2m_1 + 1) \sum_{v \in V(G_2) \setminus \{a_2\}} d(v | G_2) d(a_2, v | G_2) \\ &\quad + 2(m_1 + m_2 + 2m_1 m_2) + 1. \end{aligned}$$

Now, the formula of $S^*(G)$ is obtained by adding S_1 , S_2 and S_3 and simplifying the resulting expression. \square

In the following lemmas, the degree of an arbitrary edge of $(G_1 \sim G_2)(a_1, a_2)$ and the distances d_0 and d_4 between two arbitrary edges of this graph are computed. The results are direct consequences of Lemmas 3.7 and 3.8, respectively, so their proofs are omitted.

Lemma 3.10 *Let $e \in E((G_1 \sim G_2)(a_1, a_2))$. Then*

$$d(e|(G_1 \sim G_2)(a_1, a_2)) = \begin{cases} d(e|G_1) & e \in E(G_1), a_1 \notin V(e), \\ d(e|G_1) + 1 & e \in E(G_1), a_1 \in V(e), \\ d(e|G_2) & e \in E(G_2), a_2 \notin V(e), \\ d(e|G_2) + 1 & e \in E(G_2), a_2 \in V(e), \\ \alpha_1 + \alpha_2 & e = a_1 a_2. \end{cases}$$

Lemma 3.11 *Let $G = (G_1 \sim G_2)(a_1, a_2)$ and $e, f \in E(G)$. Then*

$$(i) \quad d_0(e, f|G) = \begin{cases} d_0(e, f|G_1) & e, f \in E(G_1), \\ d_0(e, f|G_2) & e, f \in E(G_2), \\ D_1(a_1, e|G_1) + 1 & e \in E(G_1), f = a_1 a_2, \\ D_1(a_2, e|G_2) + 1 & e \in E(G_2), f = a_1 a_2, \\ D_1(a_1, e|G_1) + D_1(a_2, f|G_2) + 2 & e \in E(G_1), f \in E(G_2), \end{cases}$$

$$(ii) \quad d_4(e, f|G) = \begin{cases} d_4(e, f|G_1) & e, f \in E(G_1), \\ d_4(e, f|G_2) & e, f \in E(G_2), \\ D_2(a_1, e|G_1) + 1 & e \in E(G_1), f = a_1 a_2, \\ D_2(a_2, e|G_2) + 1 & e \in E(G_2), f = a_1 a_2, \\ D_2(a_1, e|G_1) + D_2(a_2, f|G_2) + 1 & e \in E(G_1), f \in E(G_2). \end{cases}$$

In the following theorem, the first and second edge-modified Schultz indices of $(G_1 \sim G_2)(a_1, a_2)$ are computed.

Theorem 3.12 *The first and second edge-modified Schultz indices of $G = (G_1 \sim G_2)(a_1, a_2)$ are given by*

$$(i) \quad (W_*)_{e_0}(G) = (W_*)_{e_0}(G_1) + (W_*)_{e_0}(G_2) + \sum_{e, f \in E(G_1); a_1 \in V(e) \setminus V(f)} d(f|G_1) d_0(e, f|G_1) \\ + \sum_{e, f \in E(G_2); a_2 \in V(e) \setminus V(f)} d(f|G_2) d_0(e, f|G_2) \\ + (M_1(G_2) - 2m_2 + 2\alpha_2 + \alpha_1) \sum_{e \in E(G_1)} d(e|G_1) D_1(a_1, e|G_1) \\ + (M_1(G_1) - 2m_1 + 2\alpha_1 + \alpha_2) \sum_{f \in E(G_2)} d(f|G_2) D_1(a_2, f|G_2) \\ + 2(M_1(G_1) - 2m_1)(M_1(G_2) - 2m_2) + (\alpha_1 - 1)\delta(a_1|G_1) + (\alpha_2 - 1)\delta(a_2|G_2) \\ + (3\alpha_2 + \alpha_1)(M_1(G_1) - 2m_1) + (3\alpha_1 + \alpha_2)(M_1(G_2) - 2m_2) \\ + \alpha_1^3 + \alpha_2^3 + 4\alpha_1\alpha_2 - 3\binom{\alpha_1}{2} - 3\binom{\alpha_2}{2}.$$

$$\begin{aligned}
(ii) \quad (W_*)_{e_4}(G) &= (W_*)_{e_4}(G_1) + (W_*)_{e_4}(G_2) + \sum_{e,f \in E(G_1); a_1 \in V(e) \setminus V(f)} d(f|G_1)d_4(e, f|G_1) \\
&+ \sum_{e,f \in E(G_2); a_2 \in V(e) \setminus V(f)} d(f|G_2)d_4(e, f|G_2) \\
&+ (M_1(G_2) - 2m_2 + 2\alpha_2 + \alpha_1) \sum_{e \in E(G_1)} d(e|G_1)D_2(a_1, e|G_1) \\
&+ (M_1(G_1) - 2m_1 + 2\alpha_1 + \alpha_2) \sum_{f \in E(G_2)} d(f|G_2)D_2(a_2, f|G_2) \\
&+ \sum_{\{u,v\} \subseteq N(a_1|G_1)} [d(u|G_1) + d(v|G_1)]d(u, v|G_1) \\
&+ \sum_{\{u,v\} \subseteq N(a_2|G_2)} [d(u|G_2) + d(v|G_2)]d(u, v|G_2) \\
&+ (2\alpha_1 - 3) \sum_{\{u,v\} \subseteq N(a_1|G_1)} d(u, v|G_1) + (2\alpha_2 - 3) \sum_{\{u,v\} \subseteq N(a_2|G_2)} d(u, v|G_2) \\
&+ (M_1(G_1) - 2m_1)(M_1(G_2) - 2m_2) + (3\alpha_2 + \alpha_1)(M_1(G_1) - 2m_1) \\
&+ (3\alpha_1 + \alpha_2)(M_1(G_2) - 2m_2) + (\alpha_1 + \alpha_2)^2 + 3\alpha_1\alpha_2.
\end{aligned}$$

Proof We prove the second part of the theorem. The first part can be proved by a similar method. At first, we partition the sum in the formula of $(W_*)_{e_4}(G)$ into three sums as follows.

The first sum S_1 consists of contributions to $(W_*)_{e_4}(G)$ of pairs of edges from G_1 . In order to compute S_1 , we partition it into three sums S_{11} , S_{12} and S_{13} as follows.

The sum S_{11} is equal to

$$S_{11} = \sum_{\{e,f\} \subseteq E(G_1); a_1 \notin V(e) \cup V(f)} d(e|G)d(f|G)d_4(e, f|G).$$

Using Lemmas 3.10 and 3.11, we obtain

$$S_{11} = \sum_{\{e,f\} \subseteq E(G_1); a_1 \notin V(e) \cup V(f)} d(e|G_1)d(f|G_1)d_4(e, f|G_1).$$

The sum S_{12} is equal to

$$S_{12} = \sum_{\{e,f\} \subseteq E(G_1); a_1 \in V(e) \cap V(f)} d(e|G)d(f|G)d_4(e, f|G).$$

Using Lemmas 3.10 and 3.11, we obtain

$$\begin{aligned}
S_{12} &= \sum_{\{e,f\} \subseteq E(G_1); a_1 \in V(e) \cap V(f)} (d(e|G_1) + 1)(d(f|G_1) + 1)d_4(e, f|G_1) \\
&= \sum_{\{e,f\} \subseteq E(G_1); a_1 \in V(e) \cap V(f)} d(e|G_1)d(f|G_1)d_4(e, f|G_1) \\
&\quad + \sum_{\{u,v\} \subseteq N(a_1|G_1)} [d(u|G_1) + d(v|G_1)]d(u, v|G_1) \\
&\quad + (2\alpha_1 - 3) \sum_{\{u,v\} \subseteq N(a_1|G_1)} d(u, v|G_1).
\end{aligned}$$

The sum S_{13} is equal to

$$S_{13} = \sum_{e,f \in E(G_1); a_1 \in V(e) \setminus V(f)} d(e|G)d(f|G)d_4(e, f|G).$$

Using Lemmas 3.10 and 3.11, we obtain

$$\begin{aligned}
S_{13} &= \sum_{e,f \in E(G_1); a_1 \in V(e) \setminus V(f)} (d(e|G_1) + 1)d(f|G_1)d_4(e, f|G_1) \\
&= \sum_{e,f \in E(G_1); a_1 \in V(e) \setminus V(f)} d(e|G_1)d(f|G_1)d_4(e, f|G_1) \\
&\quad + \sum_{e,f \in E(G_1); a_1 \in V(e) \setminus V(f)} d(f|G_1)d_4(e, f|G_1).
\end{aligned}$$

By adding S_{11} , S_{12} and S_{13} , we obtain

$$\begin{aligned}
S_1 &= (W_*)_{e_4}(G_1) + \sum_{\{u,v\} \subseteq N(a_1|G_1)} [d(u|G_1) + d(v|G_1)]d(u, v|G_1) \\
&\quad + (2\alpha_1 - 3) \sum_{\{u,v\} \subseteq N(a_1|G_1)} d(u, v|G_1) + \sum_{e,f \in E(G_1); a_1 \in V(e) \setminus V(f)} d(f|G_1)d_4(e, f|G_1).
\end{aligned}$$

The second sum S_2 consists of contributions to $(W_*)_{e_4}(G)$ of pairs of edges from G_2 . Using the same argument as in the computation of S_1 , we obtain

$$\begin{aligned}
S_2 &= (W_*)_{e_4}(G_2) + \sum_{\{u,v\} \subseteq N(a_2|G_2)} [d(u|G_2) + d(v|G_2)]d(u, v|G_2) \\
&\quad + (2\alpha_2 - 3) \sum_{\{u,v\} \subseteq N(a_2|G_2)} d(u, v|G_2) + \sum_{e,f \in E(G_2); a_2 \in V(e) \setminus V(f)} d(f|G_2)d_4(e, f|G_2).
\end{aligned}$$

The third sum S_3 is taken over all pairs $\{e, f\}$ of edges in G such that $e \in E(G_1)$ and $f = a_1a_2$. In order to compute S_3 , we partition it into two sums S_{31} and S_{32} as follows.

The sum S_{31} is equal to

$$S_{31} = \sum_{e \in E(G_1); a_1 \notin V(e), f = a_1a_2} d(e|G)d(f|G)d_4(e, f|G).$$

Using Lemmas 3.10 and 3.11, we obtain

$$\begin{aligned} S_{31} &= \sum_{e \in E(G_1); a_1 \notin V(e)} d(e | G_1)(\alpha_1 + \alpha_2)[D_2(a_1, e | G_1) + 1] \\ &= (\alpha_1 + \alpha_2) \left[\sum_{e \in E(G_1)} d(e | G_1)D_2(a_1, e | G_1) + M_1(G_1) - 2m_1 - 2\alpha_1(\alpha_1 - 2) - 2\delta(a_1 | G_1) \right]. \end{aligned}$$

The sum S_{32} is equal to

$$S_{32} = \sum_{e \in E(G_1); a_1 \in V(e), f = a_1 a_2} d(e | G)d(f | G)d_4(e, f | G).$$

Using Lemmas 3.10 and 3.11, we obtain

$$S_{32} = 2 \sum_{e \in E(G_1); a_1 \in V(e)} (d(e | G_1) + 1)(\alpha_1 + \alpha_2) = 2(\alpha_1 + \alpha_2)[\alpha_1(\alpha_1 - 2) + \delta(a_1 | G_1) + \alpha_1].$$

By adding S_{31} and S_{32} , we obtain

$$S_3 = (\alpha_1 + \alpha_2) \left[\sum_{e \in E(G_1)} d(e | G_1)D_2(a_1, e | G_1) + M_1(G_1) - 2m_1 + 2\alpha_1 \right].$$

The fourth sum S_4 is taken over all pairs $\{e, f\}$ of edges in G such that $e \in E(G_2)$ and $f = a_1 a_2$. Using the same argument as in the computation of S_3 , we obtain

$$S_4 = (\alpha_1 + \alpha_2) \left[\sum_{e \in E(G_2)} d(e | G_2)D_2(a_2, e | G_2) + M_1(G_2) - 2m_2 + 2\alpha_2 \right].$$

The fifth sum S_5 is taken over all pairs $\{e, f\}$ of edges in G such that $e \in E(G_1)$ and $f \in E(G_2)$. In order to compute S_5 , we partition it into four sums S_{51} , S_{52} , S_{53} and S_{54} as follows.

The sum S_{51} is equal to

$$S_{51} = \sum_{e \in E(G_1); a_1 \notin V(e)} \sum_{f \in E(G_2); a_2 \notin V(f)} d(e | G)d(f | G)d_4(e, f | G).$$

Using Lemmas 3.10 and 3.11, we obtain

$$\begin{aligned} S_{51} &= \sum_{e \in E(G_1); a_1 \notin V(e)} \sum_{f \in E(G_2); a_2 \notin V(f)} d(e | G_1)d(f | G_2)[D_2(a_1, e | G_1) + D_2(a_2, f | G_2) + 1] \\ &= [M_1(G_2) - 2m_2 - \alpha_2(\alpha_2 - 2) - \delta(a_2 | G_2)] \\ &\quad \left[\sum_{e \in E(G_1)} d(e | G_1)D_2(a_1, e | G_1) - \alpha_1(\alpha_1 - 2) - \delta(a_1 | G_1) \right] \\ &\quad + [M_1(G_1) - 2m_1 - \alpha_1(\alpha_1 - 2) - \delta(a_1 | G_1)] \end{aligned}$$

$$\begin{aligned} & \times \left[\sum_{f \in E(G_2)} d(f|G_2)D_2(a_2, f|G_2) - \alpha_2(\alpha_2 - 2) - \delta(a_2|G_2) \right] \\ & + \left[M_1(G_1) - 2m_1 - \alpha_1(\alpha_1 - 2) - \delta(a_1|G_1) \right] \times \left[M_1(G_2) - 2m_2 - \alpha_2(\alpha_2 - 2) - \delta(a_2|G_2) \right]. \end{aligned}$$

The sum S_{52} is equal to

$$S_{52} = \sum_{e \in E(G_1); a_1 \notin V(e)} \sum_{f \in E(G_2); a_2 \in V(f)} d(e|G)d(f|G)d_4(e, f|G).$$

Using Lemmas 3.10 and 3.11, we obtain

$$\begin{aligned} S_{52} &= \sum_{e \in E(G_1); a_1 \notin V(e)} \sum_{f \in E(G_2); a_2 \in V(f)} d(e|G_1)(d(f|G_2) + 1) [D_2(a_1, e|G_1) + 2] \\ &= [\alpha_2(\alpha_2 - 1) + \delta(a_2|G_2)] \left[\sum_{e \in E(G_1)} d(e|G_1)D_2(a_1, e|G_1) - \alpha_1(\alpha_1 - 2) - \delta(a_1|G_1) \right] \\ &\quad + 2(M_1(G_1) - 2m_1 - \alpha_1(\alpha_1 - 2) - \delta(a_1|G_1)). \end{aligned}$$

The sum S_{53} is equal to

$$S_{53} = \sum_{e \in E(G_1); a_1 \in V(e)} \sum_{f \in E(G_2); a_2 \notin V(f)} d(e|G)d(f|G)d_4(e, f|G).$$

Using the same argument as in the computation of S_{52} , we obtain

$$\begin{aligned} S_{53} &= [\alpha_1(\alpha_1 - 1) + \delta(a_1|G_1)] \left[\sum_{f \in E(G_2)} d(f|G_2)D_1(a_2, f|G_2) - \alpha_2(\alpha_2 - 2) - \delta(a_2|G_2) \right] \\ &\quad + 2(M_1(G_2) - 2m_2 - \alpha_2(\alpha_2 - 2) - \delta(a_2|G_2)). \end{aligned}$$

The sum S_{54} is equal to

$$S_{54} = \sum_{e \in E(G_1); a_1 \in V(e)} \sum_{f \in E(G_2); a_2 \in V(f)} d(e|G)d(f|G)d_4(e, f|G).$$

Using Lemmas 3.10 and 3.11, we obtain

$$\begin{aligned} S_{54} &= 3 \sum_{e \in E(G_1); a_1 \in V(e)} \sum_{f \in E(G_2); a_2 \in V(f)} (d(e|G_1) + 1)(d(f|G_2) + 1) \\ &= 3[\alpha_1(\alpha_1 - 1) + \delta(a_1|G_1)] [\alpha_2(\alpha_2 - 1) + \delta(a_2|G_2)]. \end{aligned}$$

By adding S_{51} , S_{52} , S_{53} and S_{54} , we obtain

$$\begin{aligned} S_5 &= (M_1(G_2) - 2m_2 + \alpha_2) \sum_{e \in E(G_1)} d(e|G_1)D_2(a_1, e|G_1) \\ &\quad + (M_1(G_1) - 2m_1 + \alpha_1) \sum_{f \in E(G_2)} d(f|G_2)D_2(a_2, f|G_2) \end{aligned}$$

$$\begin{aligned}
&+ (M_1(G_1) - 2m_1)(M_1(G_2) - 2m_2) + 2\alpha_2(M_1(G_1) - 2m_1) \\
&+ 2\alpha_1(M_1(G_2) - 2m_2) + 3\alpha_1\alpha_2.
\end{aligned}$$

The formula of $(W_*)_{e_4}(G)$ is obtained by adding S_1, S_2, S_3, S_4 and S_5 and simplifying the resulting expression. \square

References

- [1] A.R.Ashrafi, A.Hamzeh and S.Hosseinzadeh, Calculation of some topological indices of splices and links of graphs, *J. Appl. Math. Inf.*, 29 (2011), 327–335.
- [2] M.Azari, Sharp lower bounds on the Narumi-Katayama index of graph operations, *Appl. Math. Comput.*, 239C (2014), 409–421.
- [3] M.Azari, A note on vertex-edge Wiener indices, *Iranian J. Math. Chem.*, 7(1) (2016), 11–17.
- [4] M.Azari and F.Falahati-Nezhad, On vertex-degree-based invariants of link of graphs with application in dendrimers, *J. Comput. Theor. Nanosci.*, 12(12) (2015), 5611–5616.
- [5] M.Azari and A.Iranmanesh, Edge-Wiener type invariants of splices and links of graphs, *Politehn. Univ. Bucharest Sci. Bull. Ser. A Appl. Math. Phys.*, 77(3) (2015), 143–154.
- [6] M.Azari, A.Iranmanesh and I.Gutman, Zagreb indices of bridge and chain graphs, *MATCH Commun. Math. Comput. Chem.*, 70 (2013), 921–938.
- [7] M.V.Diudea, *QSPR/QSAR Studies by Molecular Descriptors*, NOVA, New York, 2001.
- [8] T.Došlić, Splices, links and their degree-weighted Wiener polynomials, *Graph Theory Notes N. Y.*, 48 (2005), 47–55.
- [9] I.Gutman, Selected properties of the Schultz molecular topological index, *J. Chem. Inf. Comput. Sci.*, 34 (1994), 1087–1089.
- [10] I.Gutman and O.E.Polansky, *Mathematical Concepts in Organic Chemistry*, Springer, Berlin, 1986.
- [11] I.Gutman and N.Trinajstić, Graph theory and molecular orbitals, Total π -electron energy of alternant hydrocarbons, *Chem. Phys. Lett.*, 17 (1972), 535–538.
- [12] M.A.Hosseinzadeh, A.Iranmanesh and T.Došlić, On the Narumi-Katayama index of composite graphs, *Croat. Chem. Acta*, 86(4) (2013), 503–508.
- [13] A.Iranmanesh and M.Azari, The first and second Zagreb indices of several interesting classes of chemical graphs and nanostructures, In: M. V. Putz, O. Ori (Eds.), *Exotic Properties of Carbon Nanomatter*, Springer Netherlands, Dordrecht, vol. 8, 2015, pp. 153–183.
- [14] A.Iranmanesh, O.Khormali and A.Ahmadi, Generalized edge-Schultz indices of some graphs, *MATCH Commun. Math. Comput. Chem.*, 65 (2011), 93–112.
- [15] O.Khormali, A.Iranmanesh, I.Gutman and A.Ahmadi, Generalized Schultz index and its edge versions, *MATCH Commun. Math. Comput. Chem.*, 64 (2010), 783–798.
- [16] M.Mogharrab and I.Gutman, Bridge graphs and their topological indices, *MATCH Commun. Math. Comput. Chem.*, 69 (2013), 579–587.

- [17] H.P.Schultz, Topological organic chemistry 1. Graph theory and topological indices of alkanes, *J. Chem. Inf. Comput. Sci.*, 29 (1989), 227–228.
- [18] R.Sharafdini and I. Gutman, Splice graphs and their topological indices, *Kragujevac J. Sci.*, 35 (2013), 89–98.
- [19] H.Wiener, Structural determination of paraffin boiling points, *J. Am. Chem. Soc.*, 69 (1947), 17–20.
- [20] H.Wiener, Correlation of heats of isomerization and differences in heats of vaporization of isomers among the paraffin hydrocarbons, *J. Am. Chem. Soc.*, 69 (1947), 2636–2638.