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MODIFIED ZAGREB INDICES OF BRIDGE GRAPHS

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ABSTRACT

The first and the second modified Zagreb indices are defined as

$^{m}M_1(G) = \sum_{v\in V(G)} \frac{1}{(d(v))^2}$ *and* $^{m}M_2(G) = \sum_{uv\in(G)} \frac{1}{d(u)d(v)}$, *where d(v) is the degree of the vertex v in G. In this work, we obtain first and the second modified Zagreb indices of bridge graphs. Using these results, modified Zagreb indices of chemical graphs are computed.*

Keywords: *First modified Zagreb Index; Second modified Zagreb Index; Bridge graph.*

2000 Mathematics subject classification: *05C07, 05C12.*

1. INTRODUCTION

Zagreb indices are important topological indices in mathematical chemistry. The Zagreb indices have been introduced by Gutman and Trinajstic in [6] and elaborated in [5]. For a graph G = (V(G), E(G)), the first and the and the second Zagreb indices were defined as $M_1(G) = \sum_{v\in V(G)} (d(v))^2$ and $M_2(G) = \sum_{uv\in E(G)} d(u)d(v)$ respectively, where d(v) denotes the degree of the vertex v in G. In addition to the original Zagreb in dices thereof were also introduced and studied in [3, 4, 7, 12, 14-16]. Nikolic et al. introduced modified Zagreb indices in [13]. The first and the second modified Zagreb index were defined as $^{m}M_1(G) = \sum_{n\in V(G)} \frac{1}{(d(v))^2}$ and $^{m}M_2(G) = \sum_{uv\in E(G)} d(u)d(v)$, where d(v) is the degree of the vertex v in G. Hao studied the relation between the Zagreb indices and the modified Zagreb indices [8] and studied the modified Zagreb indices of Nanotubes and Dendrimer Nanostars in [9].

Some topological indices of bridge and chain graphs have been computed. Previously [1, 10, 11]. In this work, we obtain modified Zagreb indices of bridge graphs. Using these results, modified Zagreb indices of chemical graphs are computed.

In this paper, we consider connected finite graphs without loops or multiple edges. For a graph G = (V(G), E(G)), the degree of a vertex of G is the number of edges adjacent to v and it is denoted by $d_G(v)$ or simply d(v). The set of neighbours of v is denoted by N (v). For other notations in graph theory, may be consulted [2].

We can recall the definitions of bridge and chain graphs. Let $\{G_i\}_{i=1}^{k}$ be a set of finite pair-wise disjoint graphs with distinct vertices $u_i, v_i \in V(G_i)$ such that u_i and v_i are not adjacent in G_i. The bridge graph B_1 = B=1 ($G_1, G_2, \ldots, G_k; u_1, v_1, u_2, v_2, u_3, v_3, \ldots, u_k, v_k$) of $\{G_i\}_{i=1}^{k}$ with respect to the vertices $\{u_i v_i\}_{i=1}^{k}$ is the graph obtained from the graphs $G_1, G_2, \ldots, G_k$ by connecting the vertices v_i and u_{i+1} by an edge for all i = 1, 2, ...,, k-1 as shown in the figure 1.

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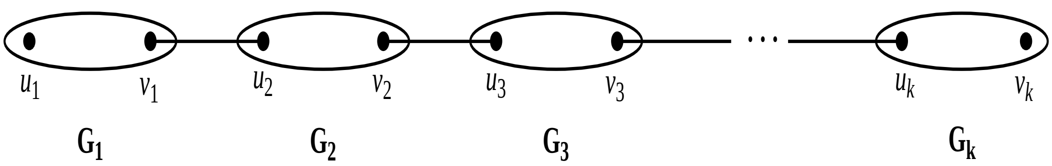

Figure-1: The bridge graph $B_1 = B_1$ (G_1, G_2, ..., Gk; u_1, v_1, u_2, v_2, ..., u_k, v_k)

Let $\{G_i\}_{i=1}^{k}$ be a set of finite pair wise disjoint graphs with vertices $v_i \in V(G_i)$. The bridge graph $B_2 = B_2(G_1, G_2, ...,, G_k;$ $v_1, v_2, v_3,...., v_k)$ of $\{G_i\}_{i=1}^{k}$ with respect to the vertices $\{v_i\}_{i=1}^{k}$ is the graph obtained form the graphs G_1, G_2,....G_k by connecting the vertices v_i and v_{i+1} is the graph obtained form the graphs G_1,G_2,....., G_k by connecting the vertices v_i and v_{i+1} by an edge for all i = 1, 2,...., k -1 as shown in the figure 2.

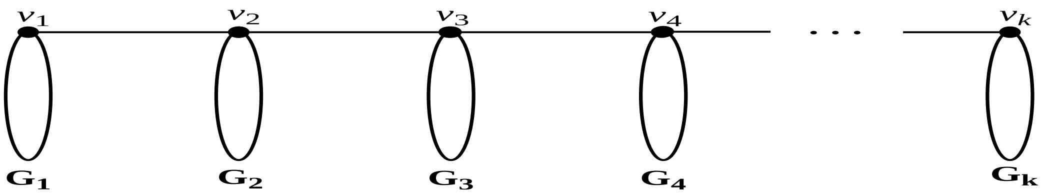

Figure-2: $B_2 = B_2$ (G_1, G_2, ..., G_k; v_1,v_2, v_3, ..., v_k).

2. MODIFIED ZAGREB INDICES OF BRIDGE GRAPH B_1

In this section, we compute first and second modified Zagreb indices of the bridge graph B_1.

Theorem 2.1: The first modified Zagreb index of the bridge graph B_1, K ≥2 is given by

$$ {}^{m}M_1(B_1) = \sum_{i=1}^{k}({}^{m}M_1(G_i)) - \left\{ \sum_{i=1,k} \frac{2d(u_i)+1}{d(u_i)^2(d(u)_i+1)^2} \right.$$
$$\left. +4\sum_{i=2}^{k-1}\left\{ \frac{d(u_i)+1}{d(u_i)^2(d(u_i)+2)^2} + \frac{d(v_i)+1)}{d(v_i)^2(d(v_i)+2)^2} \right\} \right\}$$

Proof: Using the definition of first modified Zagreb index, we have

$$ {}^{m}M_1(B_1) = \sum_{i=1}^{k} {}^{m}M_1(G_i)) - \sum_{i=1}^{k-1}\frac{1}{d(v_i)^2} - \sum_{i=2}^{k}\frac{1}{d(v_i)^2}\frac{1}{(d(v_i)+2^{\ 2})}$$
$$ + \sum_{i=2}^{k-1}\frac{1}{d(\mathrm{u}_i+2)^2} + \frac{1}{(d(v_1)+1)^2} + \frac{1}{(d(\mathrm{u}_k)+1)^2}$$

$$ = \sum_{i=1}^{k} {}^{m}M_1(G_i)) - \{ \frac{2d(v_1)+1}{d(v_1)^2(d(v_1)+1)^2} - \frac{2d(u_k)+1}{d(u_k)^2(d(u_k)+1)^2}$$

$$ +4\sum_{i=2}^{k-1}\left\{ \frac{d(u_i)+1}{d(u_i)^2(d(u_i)+2)^2} + \frac{d(v_i)+1)}{d(v_i)^2(d(v_i)+2)^2} \right\}\right\}$$

Corollary 2.1: If $G_i = G$ for all i = 1,2 ,..., k and u, v∈V(G), then

$$ {}^{m}M_1(B_1) = K\,{}^{m}M_1(G) - \left\{ \frac{2d(u)+1}{d(v_i)^2 d(u)+1^2} + \frac{2d(v)+1}{d(v)^2(d(v)+1)^2} \right.$$
$$\left. + 4\ (\mathrm{k}\ {-2}) \left\{ \frac{d(u_i)+1}{d(u_i)^2(d(u_i)+2)^2} + \frac{d(v_i)+1)}{d(v_i)^2(d(v_i)+2)^2} \right\} \right\}$$

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Theorem 2.2: The second modified Zagreb index of the bridge graph B_1, $k \geq 2$ is given by

$$ {}^{m}M_2(B_1) = \sum_{i=1}^{k}\left({}^{m}M_2(G_i)\right) - \left\{ \sum_{i=1}^{k-1} \sum_{w\in N(v_i)} \frac{1}{d(v_i)[d(v_i)+1]d(w)} + \sum_{i=2}^{k} \sum_{w\in N(u_i)} \frac{1}{d(u_i)[d(u_i)+1]d(w)} - \sum_{i=1}^{k-1} \frac{1}{[d(v_i)+1][d(u_{i+1})+1]} \right\} $$

Proof: By the definition of second modified Zagreb index, ${}^{m}M_2(B_2)$ is equal to the sum of $\frac{1}{d_{B_2}(x)d_{B_2}(y)}$, where the summation is taken over all edges $xy \in E(B_2)$. From the definition of the bridge graph B_1,
$E(B_1) = E(G_1) \cup E(G_2) \cup ... \cup E(G_k) \cup \{v_iu_{i+1}; 1 \leq i \leq k-1\}$. In order to compute ${}^{m}M_2(B_1)$, we partition our sum into four sums as follows.

The first sum S_1 is taken over all edges $xy \in E(G_1)$.

$$ S_1 = {}^{m}M_2(G_1) - \sum_{w\in N(v_1)} \frac{1}{d(v_1)d(w)} + \sum_{w\in N(v_1)} \frac{1}{(d(v_1)+1)d(w)} $$

$$ = {}^{m}M_2(G_1) - \sum_{w\in N(v_1)} \frac{1}{d(v_1)(d(v_1)+1)d(w)} $$

The second sum S_2 is taken over all edges $xy \in E(G_k)$.

$$ S_2 = {}^{m}M_2(G_k) - \sum_{w\in N(u_k)} \frac{1}{d(u_k)d(w)} + \sum_{w\in N(u_k)} \frac{1}{(d(u_k)+1)d(w)} $$

$$ = {}^{m}M_2(G_1) - \sum_{w\in N(u_k)} \frac{1}{d(u_k)(d(u_k)+1)d(w)} $$

The third sum S_3 is taken over all edges $xy \in E(G_i)$ for all $i = 2,3,...,k-1$.

$$ S_3 = \sum_{i=2}^{k-1}\left({}^{m}M_2(G_i)\right) - \sum_{i=2}^{k-1}\left\{ \sum_{w\in N(u_i)} \frac{1}{d(u_i)(d(u_i)+1)d(w)} + \sum_{w\in N(v_i)} \frac{1}{d(v_i)(d(v_i)+1)d(w)} \right\} $$

The last sum S_4 is taken over all edges v_iu_{i+1} for all $i = 1, 2, ..., k-1$.

$$ S_4 = \sum_{i=1}^{k-1} \frac{1}{(d(v_i)+1)(d(u_{i+1}+1)} $$

Now ${}^{m}M_2(B_1)$ is obtained by adding S_1, S_2, S_3, S_4.

Corollary 2.2: If $G_i = G$ for all $i = 1, 2, ..., k$ and $u, v \in V(G)$, then

$$ {}^{m}M_2(B_1) = k\left({}^{m}M_2(G)\right) - (k-1)\left\{ \sum_{w\in N(u)} \frac{1}{[d(u)][d(u)+1]d(w)} + \sum_{w\in N(v)} \frac{1}{[d(v)][d(v)+1]d(w)} - \frac{1}{[d(u)+1][d(v)+1]} \right\} $$

3. MODIFIED ZAGREB INDICES OF BRIDGE GRAPH B_2

In this section, we compute first and second modified Zagreb indices of the bridge graph B_2.

Theorem 3.1: The first modified Zagreb index of the bridge graph B_2, $k \geq 2$ is given by

$$ {}^{m}M_1(B_2) = \sum_{i=1}^{k} H(G_i) - \left\{ \sum_{i=1}^{k} \frac{1}{[d(v_i)^2]} + \sum_{i=2}^{k-1} \frac{1}{[d(v_i)+2\ ^2]} + \sum_{i=1,k}^{v} \frac{1}{[d(v_i)+1]^2} \right\} $$

Proof: Using the definition of first modified Zagreb index, we have

$$M_1(B_2) = \sum_{i=1}^{k}\left({}^{m}M_1(G_i)\right) - \left\{ \sum_{i=1}^{k}\frac{1}{[d(v_i)^2]} + \sum_{i=2}^{k-1}\frac{1}{[d(v_i)+2]^2} + \sum_{i=1,k}\frac{1}{[d(v_i)+1]^2} \right\}$$

Corollary 3.1: If $G_i = G$ for all i = 1, 2, ..., k and u, v $\in$ V(G), then

$${}^{m}M_1(B_2) = k\,{}^{m}M_1(G) - \left\{ \frac{k}{[d(v)^2]} + \frac{k-2}{[d(v)+2]^2} + \frac{2}{[d(v)+1]^2} \right\}$$

Theorem 3.2: The second modified Zagreb index of the bridge graph B_2, $k \geq 2$ is given by

$$\begin{aligned} {}^{m}M_2(B_2) = \sum_{i=1}^{k}\left({}^{m}M_2(G_i)\right) - \Bigg\{ & \sum_{i=1,k}\sum_{w\in N(v_i)}\frac{1}{d(v_i)(d(v_i)+1)d(w)} \\ & + \left\{ \sum_{i=2}^{k-1}\sum_{w\in N(v_i)}\frac{1}{d(v_i)(d(v_i)+2)d(w)} - \frac{1}{(d(v_i)+1)(d(v_i)+2)} \right\} \\ & - \left\{ \sum_{i=2}^{k-1}\frac{1}{(d(v_i)+2)(d(v_{i+1})+2)} - \frac{1}{(d(v_{k-1})+2)(d(v_k)+1)} \right\} \Bigg\} \end{aligned}$$

Proof: By the definition of second modified Zagreb index, ${}^{m}M_2(B_2)$ is equal to the sum of $\frac{2}{d_{B_2}(x)d_{B_2}(y)}$, where the summation is taken over all edges xy $\in E(B_2)$. From the definition of the bridge graph B_2, $E(B_2) = E(G_1) \cup E(G_2) \cup \ldots \cup E(G_k) \cup \{v_iu_{i+1};\ 1 \leq i \leq k-1\}$. In order to compute ${}^{m}M_2(B_2)$, we partition our sum into four sum as follows.

The first sum S_1 is taken over all edges xy $\in E(G_1)$.

$$\begin{aligned} S_1 &= {}^{m}M_2(G_1) - \sum_{w\in N(v_1)}\frac{1}{d(v_1)d(w)} + \sum_{w\in N(v_1)}\frac{1}{(d(v_1)+1)d(w)} \\ &= {}^{m}M_2(G_1) - \sum_{w\in N(v_1)}\frac{1}{d(v_1)(d(v_1)+1)d(w)} \end{aligned}$$

The second sum S_2 is taken over all edges xy $\in E(G_k)$.

$$\begin{aligned} S_2 &= {}^{m}M_2(G_k) - \sum_{w\in N(v_k)}\frac{1}{d(u_k)d(w)} + \sum_{w\in N(v_k)}\frac{1}{(d(u_k)+1)d(w)} \\ &= {}^{m}M_2(G_1) - \sum_{w\in N(v_k)}\frac{1}{d(u_k)(d(u_k)+1)d(w)} \end{aligned}$$

The third sum S_3 is taken over all edges xy $\in E(G_i)$ for all i = 2, 3, ..., k-1

$$S_3 = \sum_{i=2}^{k-1}\left\{ \sum_{w\in N(v_i)}\frac{2}{d(v_i)(d(v_i)+2)d(w)} \right\}$$

The last sum S_4 is taken over all edges v_iu_{i+1} for all i = 1, 2, ..., k – 1.

$$S_4 = \frac{1}{(d(v_1)+1)(d(v_2)+2)} + \frac{1}{(d(v_{k-1})+2)(d(v_k)+1)} + \sum_{i=1}^{k-2}\frac{1}{(d(v_i)+2)(d(v_{i+1})+2)}$$

Now ${}^{m}M_2(B_2)$ is obtained by adding S_1, S_2, S_3, S_4.

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Corollary 3.2: If $G_i = G$ for all i = 1, 2, ..., k and u, v $\in$ V(G), then

$$^{m}M_2(B_2) = k\left({}^{m}M_2(G)\right) - \left\{2\sum_{w\in N(v)} \frac{1}{d(v)(d(v)+1)d(w)} + (k-2)\right.$$
$$\left.\left\{\sum_{w\in N(v)} \frac{1}{d(v)(d(v)+2)d(w)} - \frac{1}{(d(v)+2)}\left[\frac{k-2}{(d(v)+2)} + \frac{2}{d(v)+1}\right]\right\}\right\}$$

4. APPLICATION

In this section, we consider some simple molecular graphs and determine their modified Zagreb indices.

Two vertices u and v of a hexagon H are said to be in ortho-position if they are adjacent in H. If two vertices u and v are at distance two, they are said to be in meta-position and if two vertices u and v are at distance three, they are said to be in para-position. Examples of vertices in the above three types of position are shown in figure 3.

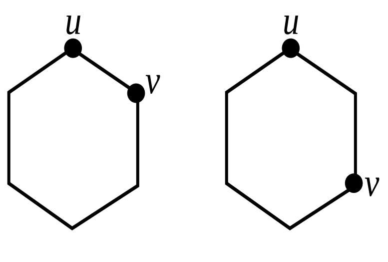

Figure-3: Ortho-, meta- and para-positions of vertices in hexagon

An internal hexagon H in a polyphenyl chain is said to be an ortho-hexagon, meta-hexagon and para-hexagon, respectively if two vertices of H incident with two edges which connect other two hexagons are in ortho-, meta- and para-position. A polyphenyl chain of h nexagons is ortho – PPC_h, denoted by O_h, if all its internal hexagons are ortho-hexagons. Similarly we define meta – PPC_h (denoted by M_h) and para – PPC_h (denoted by L_h), (see figure 4). The polyphenyl chains M_h and L_h can be viewed as the bridge graphs $B_1(C_6, C_6, ..., C_6; u, v, u, v, ..., u, v)$ (h times) where C_6 is the cycle on six vertices and u and v are the vertices shown in figure 3. Since ${}^{m}M_1(C_6)$ = ${}^{m}M_2(C_6)$ = 3/2, using corollaries 2.1 and 2.2 we obtain ${}^{m}M_1(M_h) = H\,{}^{m}M_1(L_h) = \frac{69h+22}{48}$ and ${}^{m}M_2(M_h)$ = $H\,{}^{m}M_2(L_h)$ = $\frac{23h+4}{18}$.
The polyphenyl chains O_h can be viewed as the bridge graph $B_2(C_6, C_6, ..., C_6; v, v, ..., v)$ (h times). Using corollaries 3.1 and 3.2, ${}^{m}M_1(O_h)$ = $\frac{189h+14}{144}$ and ${}^{m}M_2(O_h)$ = $\frac{75h-2}{48}$.

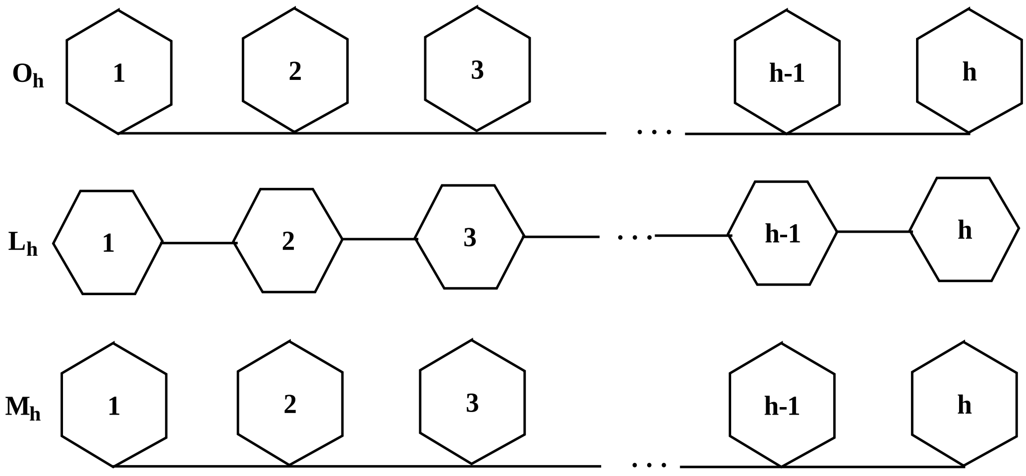

Figure-4: Ortho-, para- and meta-polyphenyl chains with h hexagons

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