

## MODIFIED ZAGREB INDICES OF BRIDGE GRAPHS

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### ABSTRACT

The first and the second modified Zagreb indices are defined as

$${}^mM_1(G) = \sum_{v \in V(G)} \frac{1}{(d(v))^2} \text{ and } {}^mM_2(G) = \sum_{uv \in E(G)} \frac{1}{d(u)d(v)}, \text{ where } d(v) \text{ is the degree of the vertex } v \text{ in } G. \text{ In this work,}$$

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 Trinajstić in [6] and elaborated in [5]. For a graph  $G = (V(G), E(G))$ , the first 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 indices 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  ${}^mM_1(G) = \sum_{v \in V(G)} \frac{1}{(d(v))^2}$  and  ${}^mM_2(G) = \sum_{uv \in E(G)} d(u)d(v)$ , 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].

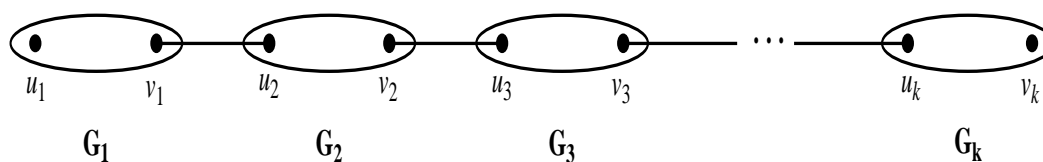
Some topological indices of bridge and chain graphs have been computed. Previously [1, 10, 11]. In this work, we obtain modified Zagreb indices of bridge graphs. Using these results, modified Zagreb indices of chemical graphs are computed.

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  $B_1 = B_1(G_1, G_2, \dots, G_k; u_1, v_1, u_2, v_2, u_3, v_3, \dots, u_k, v_k)$  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  $G_1, G_2, \dots, G_k$  by connecting the vertices  $v_i$  and  $u_{i+1}$  by an edge for all  $i = 1, 2, \dots, k-1$  as shown in the figure 1.

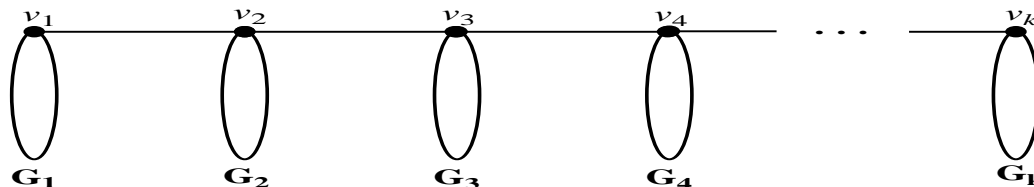
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**Figure-1:** The bridge graph  $B_1 = B_1(G_1, G_2, \dots, G_k; u_1, v_1, u_2, v_2, \dots, u_k, v_k)$

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  $B_2 = B_2(G_1, G_2, \dots, G_k; v_1, v_2, v_3, \dots, v_k)$  of  $\{G_i\}_{i=1}^k$  with respect to the vertices  $\{v_i\}_{i=1}^k$  is the graph obtained from the graphs  $G_1, G_2, \dots, G_k$  by connecting the vertices  $v_i$  and  $v_{i+1}$  by an edge for all  $i = 1, 2, \dots, k-1$  as shown in the figure 2.



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

## 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  $B_1$ ,  $K \geq 2$  is given by

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

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

$$\begin{aligned} {}^m M_1(B_1) &= \sum_{i=1}^k {}^m M_1(G_i) - \sum_{i=1}^{k-1} \frac{1}{d(v_i)^2} - \sum_{i=2}^k \frac{1}{d(v_i)^2 (d(v_i) + 2)^2} \\ &\quad + \sum_{i=2}^{k-1} \frac{1}{d(u_i + 2)^2} + \frac{1}{(d(v_i) + 1)^2} + \frac{1}{(d(u_k) + 1)^2} \\ &= \sum_{i=1}^k {}^m M_1(G_i) - \left\{ \frac{2d(v_1) + 1}{d(v_1)^2 (d(v_1) + 1)^2} - \frac{2d(u_k) + 1}{d(u_k)^2 (d(u_k) + 1)^2} \right. \\ &\quad \left. + 4 \sum_{i=2}^{k-1} \left\{ \frac{d(u_i) + 1}{d(u_i)^2 (d(u_i) + 2)^2} + \frac{d(v_i) + 1}{d(v_i)^2 (d(v_i) + 2)^2} \right\} \right\} \end{aligned}$$

**Corollary 2.1:** If  $G_i = G$  for all  $i = 1, 2, \dots, k$  and  $u, v \in V(G)$ , then

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

**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  $B_1$ ,  $E(B_1) = E(G_1) \cup E(G_2) \cup \dots \cup E(G_k) \cup \{v_i u_{i+1}; 1 \leq i \leq k-1\}$ . 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  $xy \in E(G_k)$ .

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

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

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

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

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

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  $i = 1, 2, \dots, k$  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

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

**Corollary 3.1:** If  $G_i = G$  for all  $i = 1, 2, \dots, k$  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

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

**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  $B_2$ ,  $E(B_2) = E(G_1) \cup E(G_2) \cup \dots \cup E(G_k) \cup \{v_i u_{i+1}; 1 \leq i \leq k-1\}$ . 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  $xy \in E(G_k)$ .

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

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

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

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

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

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

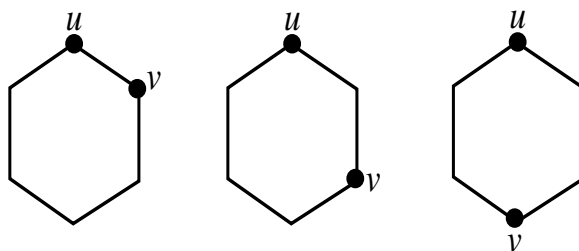
**Corollary 3.2:** If  $G_i = G$  for all  $i = 1, 2, \dots, k$  and  $u, v \in V(G)$ , then

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

#### 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.

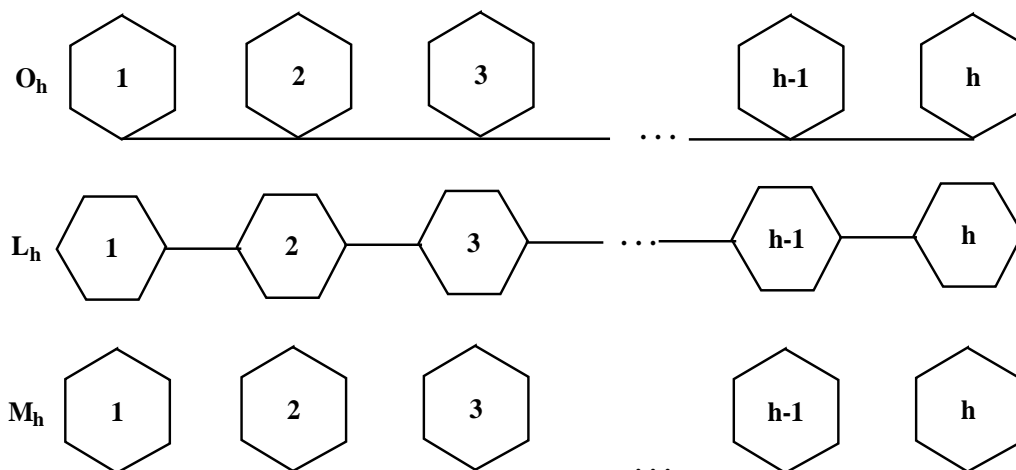


**Figure-3:** Ortho-, meta- and para-positions of vertices in hexagon

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  $h$  hexagons 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  $B_1(C_6, C_6, \dots, C_6; u, v, u, v, \dots, u, v)$  ( $h$  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  $B_2(C_6, C_6, \dots, C_6; v, v, \dots, v)$  ( $h$  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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