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Zagreb Indices of Bridge and Chain Graphs

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Abstract

We show how the first and second Zagreb indices of bridge and chain graphs are determined from the respective indices of the component graphs. The special cases when the bridge and chain graphs are built from copies of the same component are also elaborated. Using these results, the Zagreb indices of some classes of chemical graphs and nanostructures are computed.

1 Introduction

In this paper, we consider connected finite graphs without loops or multiple edges. Let G be such a graph with the vertex set $V(G)$ and the edge set $E(G)$. For $u \in V(G)$, we denote by $N_G(u)$ the set of all first neighbors of u in G. The cardinality of $N_G(u)$ is called the degree of u in G and will be denoted by $\deg_G(u)$. We denote by $\alpha_G(u)$, the sum of degrees of all neighbors of the vertex u in G, i.e., $\alpha_G(u) = \sum_{a \in N_G(u)} \deg_G(a)$. We denote by $|S|$ the cardinality of a set S.

In theoretical chemistry, the physico–chemical properties of chemical compounds are often modelled by means of molecular–graph–based structure–descriptors, which are also

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referred to as topological indices [8]. The Zagreb indices belong among the oldest topological indices, and were introduced as early as in 1972 [9,10]. For details on their theory and applications see [2–4, 7, 14, 17–19], and especially the recent papers [5, 6, 13, 15, 16]. The first and second Zagreb indices of G are denoted by $M_1(G)$ and $M_2(G)$, respectively, and are defined as:

$$M_1(G) = \sum_{u \in V(G)} \deg_G(u)^2 \qquad \text{and} \qquad M_2(G) = \sum_{uv \in E(G)} \deg_G(u) \deg_G(v) \ . \tag{1}$$

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

$$M_1(G) = \sum_{uv \in E(G)} \left[\deg_G(u) + \deg_G(v)\right] \ .$$

At this point we recall the definitions of bridge and chain graphs. Let $\{G_i\}_{i=1}^d$ be a set of finite pairwise disjoint graphs with distinct vertices $v_i, w_i \in V(G_i)$. The bridge graph $B_1 = B_1(G_1, G_2, \ldots, G_d; v_1, v_2, \ldots, v_d)$ of $\{G_i\}_{i=1}^d$ with respect to the vertices $\{v_i\}_{i=1}^d$ is the graph obtained from the graphs $G_1, G_2, \ldots, G_d$ by connecting the vertices v_i and v_{i+1} by an edge for all $i = 1, 2, \ldots, d-1$, as shown in Fig. 1.

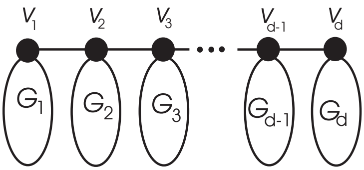

Fig. 1. The bridge graph $B_1 = B_1(G_1, G_2, \ldots, G_d; v_1, v_2, \ldots, v_d)$.

The bridge graph $B_2 = B_2(G_1, G_2, \ldots, G_d; v_1, w_1, v_2, w_2, \ldots, v_d, w_d)$ of $\{G_i\}_{i=1}^d$ with respect to the vertices $\{v_i, w_i\}_{i=1}^d$ is the graph obtained from the graphs $G_1, G_2, \ldots, G_d$ by connecting the vertices w_i and v_{i+1} by an edge for all $i = 1, 2, \ldots, d-1$, as shown in Fig. 2.

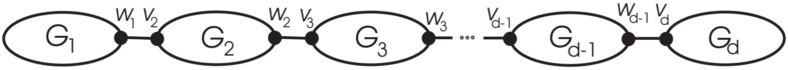

Fig. 2. The bridge graph $B_2 = B_2(G_1, G_2, \ldots, G_d; v_1, w_1, v_2, w_2, \ldots, v_d, w_d)$.

The chain graph $C = C(G_1, G_2, \ldots, G_d; v_1, w_1, v_2, w_2, \ldots, v_d, w_d)$ of $\{G_i\}_{i=1}^{d}$ with respect to the vertices $\{v_i, w_i\}_{i=1}^{d}$ is the graph obtained from the graphs $G_1, G_2, \ldots, G_d$ by identifying the vertices w_i and v_{i+1} for all $i = 1, 2, \ldots, d-1$, as shown in Fig. 3.

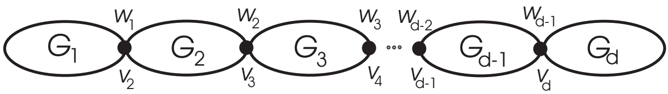

Fig. 3. The chain graph $C = C(G_1, G_2, \ldots, G_d; v_1, w_1, v_2, w_2, \ldots, v_d, w_d)$.

Some topological indices of bridge and chain graphs have been computed, previously [11, 12]. In this paper, we determine the first and second Zagreb indices for these graphs, including the important special case when the components G_i , $i = 1, 2, \ldots, d$ are mutually isomorphic. In addition, several classes of chemical graphs and nanostructures are considered.

2 Zagreb indices of the bridge graph B_1

In this section, we compute the first and second Zagreb indices of the bridge graph $B_1 = B_1(G_1, G_2, \ldots, G_d; v_1, v_2, \ldots, v_d)$ in terms of the graphs G_i. First, we state the following simple Lemma, that is crucial in this section. It follows immediately from the definition of B_1, and its proof is therefore omitted.

Lemma 2.1. *The degree of an arbitrary vertex u of the bridge graph B_1 , $d \geq 2$, is given by:*

$$\deg_{B_1}(u) = \begin{cases} \deg_{G_i}(u) & if \quad u \in V(G_i) - \{v_i\}, 1 \leq i \leq d \\ \nu_1 + 1 & if \quad u = v_1 \\ \nu_i + 2 & if \quad u = v_i \ , \ 2 \leq i \leq d-1 \\ \nu_d + 1 & if \quad u = v_d \end{cases}$$

where $\nu_i = \deg_{G_i}(v_i)$ for $1 \leq i \leq d$. ■

2.1 First Zagreb index of the bridge graph B_1

Theorem 2.2. *The first Zagreb index of the bridge graph* $B_1\,, d \geq 2$*, is given by:*

$$M_1(B_1) = \sum_{i=1}^{d} M_1(G_i) + 2\nu_1 + 4\sum_{i=2}^{d-1} \nu_i + 2\nu_d + 4d - 6 \tag{2}$$

where $\nu_i = \deg_{G_i}(v_i)$*, for* $1 \leq i \leq d$.

Proof. Using the definition of the first Zagreb index, Eq. (1), and Lemma 2.1, we have:

$$\begin{aligned} M_1(B_1) &= \sum_{i=1}^{d} \sum_{u \in V(G_i)-\{v_i\}} \deg_{G_i}(u)^2 + (\nu_1+1)^2 + \sum_{i=2}^{d-1} (\nu_i+2)^2 + (\nu_d+1)^2 \\ &= \sum_{i=1}^{d} M_1(G_i) - \sum_{i=1}^{d} \nu_i^2 + \nu_1^2 + 2\nu_1 + 1 + \sum_{i=2}^{d-1} \nu_i^2 \\ &+ \ 4\sum_{i=2}^{d-1} \nu_i + 4(d-2) + \nu_d^2 + 2\nu_d + 1 \end{aligned}$$

from which Eq. (2) follows straightforwardly. ■

Suppose that v is a vertex of a graph G, and let $G_i = G$ and $v_i = v$ for all $i = 1, 2, \ldots, d$. Using Theorem 2.2, we easily arrive at:

Corollary 2.3. *The first Zagreb index of the bridge graph* $B_1 = B_1(G, G, \ldots, G; v, \ldots, v)$*,* *(*$d \geq 2$ *times) is given by:*

$$M_1(B_1) = d\,M_1(G) + 4\nu(d-1) + 4d - 6$$

where $\nu = \deg_G(v)$. ■

2.2 Second Zagreb index of the bridge graph B_1

Theorem 2.4. *The second Zagreb index of the bridge graph* $B_1\,, d \geq 3$*, is given by:*

$$\begin{aligned} M_2(B_1) &= \sum_{i=1}^{d} M_2(G_i) + \alpha_{G_1}(v_1) + \alpha_{G_d}(v_d) + 2\sum_{i=2}^{d-1} \alpha_{G_i}(v_i) + \sum_{i=1}^{d-1} \nu_i\,\nu_{i+1} \\ &+ \ 2(\nu_1 + \nu_d) - (\nu_2 + \nu_{d-1}) + 4\sum_{i=2}^{d-1} \nu_i + 4(d-2) \end{aligned} \tag{3}$$

where $\nu_i = \deg_{G_i}(v_i)$*, for* $1 \leq i \leq d$.

Proof. By definition of the second Zagreb index, $M_2(B_1)$ is equal to the sum of $\deg_{B_1}(a)\deg_{B_1}(b)$, where summation is taken over all edges $ab \in E(B_1)$. From the definition of the bridge graph B_1, $E(B_1) = E(G_1) \cup E(G_2) \cup \ldots \cup E(G_d) \cup \{v_i v_{i+1} | 1 \le i \le d-1\}$. In order to compute $M_2(B_1)$, we partition our sum into four sums as follows:

The first sum S_1 is taken over all edges $ab \in E(G_1)$. Using Lemma 2.1,

$$\begin{aligned} S_1 &= \sum_{ab \in E(G_1)} \deg_{B_1}(a)\deg_{B_1}(b) = \sum_{ab \in E(G_1)\,;\, a,b \neq v_1} \deg_{G_1}(a)\deg_{G_1}(b) \\ &+ \sum_{ab \in E(G_1)\,;\, a \in V(G_1)\,,\; b = v_1} \deg_{G_1}(a)[\deg_{G_1}(v_1)+1] \\ &= M_2(G_1) + \alpha_{G_1}(v_1)\ . \end{aligned}$$

The second sum S_2 is taken over all edges $ab \in E(G_d)$. Using Lemma 2.1, we obtain

$$\begin{aligned} S_2 &= \sum_{ab \in E(G_d)} \deg_{B_1}(a)\deg_{B_1}(b) = \sum_{ab \in E(G_d)\,;\, a,b \neq v_d} \deg_{G_d}(a)\deg_{G_d}(b) \\ &+ \sum_{ab \in E(G_d)\,;\, a \in V(G_d), b = v_d} \deg_{G_d}(a)[\deg_{G_d}(v_d)+1] \\ &= M_2(G_d) + \alpha_{G_d}(v_d)\ . \end{aligned}$$

The third sum S_3 is taken over all edges $ab \in E(G_i)$ for all $2 \le i \le d-1$. Using Lemma 2.1,

$$\begin{aligned} S_3 &= \sum_{i=2}^{d-1} \sum_{ab \in E(G_i)} \deg_{B_1}(a)\deg_{B_1}(b) = \sum_{i=2}^{d-1} \left\{ \sum_{ab \in E(G_i)\,;\, a,b \neq v_i} \deg_{G_i}(a)\deg_{G_i}(b) \right. \\ &+ \left. \sum_{ab \in E(G_i)\,;\, a \in V(G_i)\,,\; b = v_i} \deg_{G_i}(a)[\deg_{G_i}(v_i)+2] \right\} \\ &= \sum_{i=2}^{d-1} M_2(G_i) + 2\sum_{i=2}^{d-1} \alpha_{G_i}(v_i)\ . \end{aligned}$$

The last sum S_4 is taken over all edges $v_i v_{i+1}$ for all $1 \le i \le d-1$. Using Lemma 2.1, we get:

$$\begin{aligned} S_4 &= \sum_{i=1}^{d-1} \sum_{ab = v_i v_{i+1}} \deg_{B_1}(a)\deg_{B_1}(b) \\ &= (\nu_1+1)(\nu_2+2) + \sum_{i=2}^{d-2} (\nu_i+2)(\nu_{i+1}+2) + (\nu_{d-1}+2)(\nu_d+1) \end{aligned}$$

$$
\begin{aligned}
&= \nu_1\nu_2 + 2\nu_1 + \nu_2 + 2 + \sum_{i=2}^{d-2} \nu_i\,\nu_{i+1} + 2\sum_{i=2}^{d-2} \nu_i \\
&+ \; 2\sum_{i=3}^{d-1} \nu_i + 4(d-3) + \nu_{d-1}\,\nu_d + \nu_{d-1} + 2\nu_d + 2 \\
&= \sum_{i=1}^{d-1} \nu_i\,\nu_{i+1} + 2(\nu_1 + \nu_d) - (\nu_2 + \nu_{d-1}) + 4\sum_{i=2}^{d-1} \nu_i + 4(d-2)\ .
\end{aligned}
$$

Eq. (3) is obtained by adding S_1, S_2, S_3, S_4. ■

Suppose that v is a vertex of a graph G, and let $G_i = G$ and $v_i = v$ for all $i = 1, 2, \ldots, d$.

Corollary 2.5. *The first Zagreb index of the bridge graph B_1, ($d \geq 3$ times), is given by:*

$$M_2(B_1) = dM_2(G) + (d-1)((\nu+2)^2 + 2\alpha_G(v)) - 2(\nu+2)$$

where $\nu = \deg_G(v)$. ■

3 Zagreb indices of the bridge graph B_2

In this section, we give a formula for the first and second Zagreb indices of the bridge graph $B_2 = B_2(G_1, G_2, \ldots, G_d; v_1, w_1, v_2, w_2, \ldots, v_d, w_d)$ in terms of the graphs G_i. We start this section with the following simple lemma. It follows immediately from the definition of B_2.

Lemma 3.1. *The degree of an arbitrary vertex u of the bridge graph B_2, $d \geq 2$, is given by:*

$$
\deg_{B_2}(u) = \begin{cases}
\deg_{G_1}(u) & \text{if} \quad u \in V(G_1) - \{w_1\} \\
\deg_{G_d}(u) & \text{if} \quad u \in V(G_d) - \{v_d\} \\
\deg_{G_i}(u) & \text{if} \quad u \in V(G_i) - \{v_i, w_i\}\ ,\ 2 \leq i \leq d-1 \\
\omega_i + 1 & \text{if} \quad u = w_i\ ,\ 1 \leq i \leq d-1 \\
\nu_i + 1 & \text{if} \quad u = v_i\ ,\ 2 \leq i \leq d
\end{cases}
$$

where $\nu_i = \deg_{G_i}(v_i)$, $\omega_i = \deg_{G_i}(w_i)$, for $1 \leq i \leq d$. ■

3.1 First Zagreb index of the bridge graph B_2

Theorem 3.2. *The first Zagreb index of the bridge graph B_2, $d \geq 2$, is given by:*

$$M_1(B_2) = \sum_{i=1}^{d} M_1(G_i) + 2\sum_{i=1}^{d-1} \omega_i + 2\sum_{i=2}^{d} \nu_i + 2d - 2 \tag{4}$$

where $\nu_i = \deg_{G_i}(v_i)$, $\omega_i = \deg_{G_i}(w_i)$, *for* $1 \leq i \leq d$.

Proof. Using the definition (1) of the first Zagreb index and Lemma 3.1, we have:

$$\begin{aligned} M_1(B_2) &= \sum_{u \in V(G_1)-\{w_1\}} \deg_{G_1}(u)^2 + \sum_{i=2}^{d-1} \sum_{u \in V(G_i)-\{v_i,w_i\}} \deg_{G_i}(u)^2 \\ &+ \sum_{u \in V(G_d)-\{v_d\}} \deg_{G_d}(u)^2 + \sum_{i=1}^{d-1} (\omega_i+1)^2 + \sum_{i=2}^{d} (\nu_i+1)^2 \\ &= M_1(G_1) - {\omega_1}^2 + \sum_{i=2}^{d-1} M_1(G_i) - \sum_{i=2}^{d-1} {\nu_i}^2 - \sum_{i=2}^{d-1} \omega_i^2 + M_1(G_d) - {\nu_d}^2 \\ &+ \sum_{i=1}^{d-1} \omega_i^2 + 2\sum_{i=1}^{d-1} \omega_i + d - 1 + \sum_{i=2}^{d} {\nu_i}^2 + 2\sum_{i=2}^{d} \nu_i + d - 1 \end{aligned}$$

from which Eq. (4) follows straightforwardly. ■

Suppose that v and w are two vertices of a graph G, and let $G_i = G$, $v_i = v$ and $w_i = w$ for all $i = 1, 2, \ldots, d$. Then Theorem 3.2 implies:

Corollary 3.3. *The first Zagreb index of the bridge graph* B_2 *, (*$d \geq 2$ *times), is given by:*

$$M_1(B_2) = d\, M_1(G) + 2(d-1)(\nu + \omega + 1)$$

where $\nu = \deg_G(v)$, $\omega = \deg_G(w)$. ■

3.2 Second Zagreb index of the bridge graph B_2

Theorem 3.4. *The second Zagreb index of* $B_2\,, d \geq 2$*, is given by:*

$$\begin{aligned} M_2(B_2) &= \sum_{i=1}^{d} M_2(G_i) + \sum_{i=1}^{d-1} [\omega_i + \alpha_{G_i}(w_i)] + \sum_{i=2}^{d} [\nu_i + \alpha_{G_i}(v_i)] \\ &+ \sum_{i=1}^{d-1} \omega_i\, \nu_{i+1} + d + n - 1 \end{aligned} \tag{5}$$

where $\nu_i = \deg_{G_i}(v_i)$, $\omega_i = \deg_{G_i}(w_i)$, *for* $1 \leq i \leq d$ *and* n *is the order of the graphs* $G_i\,, 2 \leq i \leq d-1$. *It is additionally assumed that the vertices* v_i *and* w_i *of* G_i *are adjacent.*

Proof. From the definition of the bridge graph B_2, $E(B_2) = E(G_1) \cup E(G_2) \cup \ldots \cup E(G_d) \cup \{w_i v_{i+1} | 1 \leq i \leq d-1\}$. Using the same argument as in the proof of Theorem 2.4, we partition the sum in the formula of $M_2(B_2)$ into five sums as follows:

The first sum S_1 is taken over all edges $ab \in E(G_1)$. Using Lemma 3.1 we have

$$\begin{aligned} S_1 &= \sum_{ab\in E(G_1)} \deg_{B_2}(a)\deg_{B_2}(b) = \sum_{ab\in E(G_1)\,;\,a,b\neq w_1} \deg_{G_1}(a)\deg_{G_1}(b) \\ &+ \sum_{ab\in E(G_1)\,;\,a\in V(G_1)\,,\,b=w_1} \deg_{G_1}(a)[\deg_{G_1}(w_1)+1] \\ &= M_2(G_1) + \alpha_{G_1}(w_1)\ . \end{aligned}$$

Analogously,

$$S_2 = M_2(G_d) + \alpha_{G_d}(v_d)$$

where S_2 is the sum over all edges $ab \in E(G_d)$,

$$S_3 = \sum_{i\in I}[M_2(G_i) + \alpha_{G_i}(v_i) + \alpha_{G_i}(w_i) + 1]$$

where $I = \{i|2 \le i \le d-1, v_iw_i \in E(G_i)\}$, and S_3 is the sum over all edges $ab \in E(G_i)$ for all $i \in I$,

$$S_4 = \sum_{i\in \bar{I}}(M_2(G_i) + \alpha_{G_i}(v_i) + \alpha_{G_i}(w_i))$$

where $\bar{I} = \{i|2 \le i \le d-1, v_iw_i \notin E(G_i)\} = \{2,3,\ldots,d-1\} - I$, and S_4 is the sum over all edges $ab \in E(G_i)$ for all $i \in \bar{I}$, and

$$S_5 = \sum_{i=1}^{d-1}\omega_i + \sum_{i=2}^{d}\nu_i + \sum_{i=1}^{d-1}\omega_i\,\nu_{i+1} + d - 1$$

where S_5 is the sum over all edges w_iv_{i+1}, $1 \le i \le d-1$.

Adding the quantities S_1, S_2, S_3, S_4, S_5, we arrive at Eq. (5). ■

Suppose that v and w are two vertices of a graph G, and let $G_i = G$, $v_i = v$ and $w_i = w$ for all $i = 1,2,\ldots,d$.

Corollary 3.5. *Let* $\nu = \deg_G(v)$ *and* $\omega = \deg_G(w)$. *If* v *and* w *are adjacent in* G, *then*

$$M_2(B_2) = d\,M_2(G) + (d-1)[\nu + \omega + \nu\,\omega + \alpha_G(v) + \alpha_G(w) + 2] - 1$$

whereas otherwise,

$$M_2(B_2) = d\,M_2(G) + (d-1)[\nu + \omega + \nu\,\omega + \alpha_G(v) + \alpha_G(w) + 1]\ . \quad ■$$

Remark 3.6. The formulas given in Theorem 2.4 and Corollary 2.5 do not hold for the case $d = 2$. Since $B_1(G_1, G_2; w_1, v_2) \equiv B_2(G_1, G_2; v_1, w_1, v_2, w_2)$, we can apply Theorem 3.4 and Corollary 3.5 to compute the second Zagreb index of the bridge graphs consisting of two components. Hence we can reproduce the result communicated by Ashrafi et al. [1].

4 Zagreb indices of chain graphs

In this section, we give a formula for the first and second Zagreb indices of the chain graph $C = C(G_1, G_2, \ldots, G_d, v_1, w_1, v_2, w_2, \ldots, v_d, w_d)$, in terms of the graphs G_i. We first state a simple Lemma which immediately follows from the definition of C.

Lemma 4.1. *The degree of an arbitrary vertex u of the bridge graph C , $d \geq 2$, is given by:*

$$\deg_C(u) = \begin{cases} \deg_{G_1}(u) & \textit{if} \quad u \in V(G_1) - \{w_1\} \\ \deg_{G_d}(u) & \textit{if} \quad u \in V(G_d) - \{v_d\} \\ \deg_{G_i}(u) & \textit{if} \quad u \in V(G_i) - \{v_i, w_i\} \ , \ 2 \leq i \leq d-1 \\ \omega_i + \nu_{i+1} & \textit{if} \quad u = w_i = v_{i+1} \ , \ 1 \leq i \leq d-1 \end{cases}$$

where $\nu_i = \deg_{G_i}(v_i)$, $\omega_i = \deg_{G_i}(w_i)$, for $1 \leq i \leq d$. ■

4.1 First Zagreb index of chain graphs

Theorem 4.2. *The first Zagreb index of the chain graph C , $d \geq 2$, is given by:*

$$M_1(C) = \sum_{i=1}^{d} M_1(G_i) + 2 \sum_{i=1}^{d-1} \omega_i \, \nu_{i+1}$$

where $\nu_i = \deg_{G_i}(v_i)$, $\omega_i = \deg_{G_i}(w_i)$, for $1 \leq i \leq d$.

Proof. Similar to the proof of Theorem 3.2 and by definition of the chain graph, we have:

$$\begin{aligned} M_1(C) &= \sum_{u \in V(G_1)-\{w_1\}} \deg_C(u)^2 + \sum_{i=2}^{d-1} \sum_{u \in V(G_i)-\{v_i, w_i\}} \deg_C(u)^2 \\ &+ \sum_{u \in V(G_d)-\{v_d\}} \deg_C(u)^2 + \sum_{i=1}^{d-1} \sum_{u=w_i=v_{i+1}} \deg_C(u)^2 \end{aligned}$$

$$= \sum_{u\in V(G_1)-\{w_1\}} \deg_{G_1}(u)^2 + \sum_{i=2}^{d-1} \sum_{u\in V(G_i)-\{v_i,w_i\}} \deg_{G_i}(u)^2$$

$$+ \sum_{u\in V(G_d)-\{v_d\}} \deg_{G_d}(u)^2 + \sum_{i=1}^{d-1}(\omega_i + \nu_{i+1})^2$$

$$= M_1(G_1) - {\omega_1}^2 + \sum_{i=2}^{d-1} M_1(G_i) - \sum_{i=2}^{d-1} \nu_i^2 - \sum_{i=2}^{d-1} {\omega_i}^2 + M_1(G_d) - {\nu_d}^2$$

$$+ \sum_{i=1}^{d-1} \omega_i^2 + \sum_{i=2}^{d} \nu_i^2 + 2\sum_{i=1}^{d-1} \omega_i\, \nu_{i+1} \ . \qquad \blacksquare$$

Suppose that v and w are two vertices of a graph G, and let $G_i = G$, $v_i = v$, and $w_i = w$ for all $i = 1, 2, \ldots, d$.

Corollary 4.3. *The first Zagreb index of the chain graph C, ($d \geq 2$ times), is given by:*

$$M_1(C) = d\, M_1(G) + 2(d-1)\nu\, \omega$$

where $\nu = \deg_G(v)$, $\omega = \deg_G(w)$. $\blacksquare$

4.2 Second Zagreb index of chain graphs

Theorem 4.4. *The second Zagreb index of the chain graph C, $d \geq 2$, is given by:*

$$M_2(C) = \sum_{i=1}^{d} M_2(G_i) + \sum_{i=1}^{d-1} [\omega_i\, \alpha_{G_{i+1}}(v_{i+1}) + \nu_{i+1}\, \alpha_{G_i}(w_i)] + \sum_{i\in I} \omega_{i-1}\, \nu_{i+1}$$

where $\nu_i = \deg_{G_i}(v_i)$, $\omega_i = \deg_{G_i}(w_i)$, *for* $1 \leq i \leq d$ *and* $I = \{i | 1 \leq i \leq d-1\,,\ v_i w_i \in E(G_i)\}$.

Proof. In a similar manner as in the proof of Theorems 2.4 and 3.4, we partition the sum in the formula of $M_2(C)$ into the four terms as follows:

The first sum S_1 is taken over all edges $ab \in E(G_1)$. Using Lemma 4.1, we get

$$S_1 = M_2(G_1) + \nu_2\, \alpha_{G_1}(w_1) \ .$$

Further,

$$S_2 = M_2(G_d) + \omega_{d-1}\, \alpha_{G_d}(v_d)$$

where S_2 is the sum over all edges $ab \in E(G_d)$,

$$S_3 = \sum_{i \in I} [M_2(G_i) + \omega_{i-1}\, \alpha_{G_i}(v_i) + \nu_{i+1}\, \alpha_{G_i}(w_i) + \omega_{i-1}\, \nu_{i+1}]$$

where S_3 is the sum over all edges $ab \in E(G_i)$ for all $i \in I$, and

$$S_4 = \sum_{i \in \bar{I}} [M_2(G_i) + \omega_{i-1}\, \alpha_{G_i}(v_i) + \nu_{i+1}\, \alpha_{G_i}(w_i)]$$

where S_4 is the sum over all edges $ab \in E(G_i)$ for all $i \in \bar{I}$.

Adding S_1, S_2, S_3, S_4, we arrive at the expression for $M_2(C)$, given in Theorem 4.4. ■

Suppose that v and w are two vertices of a graph G, and let $G_i = G$, $v_i = v$, and $w_i = w$ for all $i = 1, 2, \ldots, d$. Then from Theorem 4.4 follows:

Corollary 4.5. *Let $\nu = \deg_G(v)$ and $\omega = \deg_G(w)$. If v and w are adjacent in G, then*

$$M_2(C) = d\, M_2(G) + (d-1)[\omega\, \alpha_G(v) + \nu\, \alpha_G(w)] + (d-2)\nu\, \omega$$

whereas otherwise,

$$M_2(C) = d\, M_2(G) + (d-1)[\omega\, \alpha_G(v) + \nu\, \alpha_G(w)]\ .$$ ■

5 Examples

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

Example 5.1. Two vertices v and w of a hexagon H are said to be in ortho-position if there are adjacent in H. If two vertices v and w are at distance two, then they are said to be in meta-position, and if two vertices v and w are at distance three, then they are said to be in para-position. Examples of vertices in the above three types of positions are illustrated in Fig. 4.

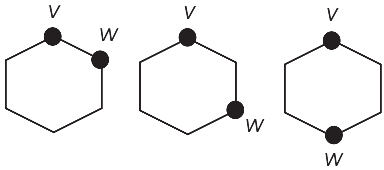

Fig. 4. Ortho-, meta- and para-positions of vertices in a hexagon.

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 and is denoted by O_h, if all its internal hexagons are ortho-hexagons. In a fully analogous manner, we define meta-PPC_h (denoted by M_h) and para-PPC_h (denoted by L_h), see Fig. 5.

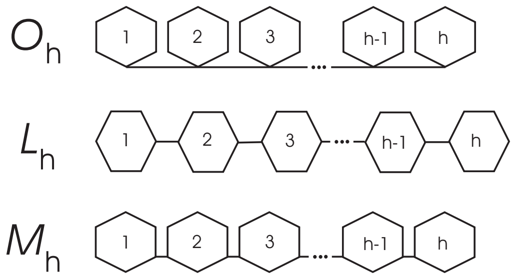

Fig. 5. Ortho-, para-, and meta-polyphenyl chains with six hexagons.

We may view the polyphenyl chains O_h , M_h , and L_h as the chain graphs $B_2(C_6, C_6, \ldots, C_6; v, w, v, w, \ldots, v, w)$ (h times) where C_6 is the cycle with six vertices and v and w are the vertices shown in Fig. 4. Since all vertices of C_6 are of degree two, it is $M_1(C_6) = M_2(C_6) = 24$, $\nu = \omega = 2$, and $\alpha_{C_6}(v) = \alpha_{C_6}(w) = 4$. Using Corollary 3.3, we obtain:

$$M_1(O_h) = M_1(M_h) = M_1(L_h) = 24h + 2(h-1)(2+2+1) = 34h - 10 \ .$$

Note that v and w are adjacent in O_h, but are not adjacent in M_h and L_h. Thus by Corollary 3.5

$$\begin{aligned} M_2(O_h) &= 24h + (h-1)(2+2+4+4+4+2) - 1 = 42h - 19 \\ M_2(M_h) &= M_2(L_h) = 24h + (h-1)(2+2+4+4+4+1) = 41h - 17 \ . \end{aligned}$$

Example 5.2. Consider the spiro-chain of the cycle C_n for arbitrary $n \geq 3$. Choosing the numbering for vertices of C_n such that the vertex v has number 1, the number i of the vertex w has to be in $\{2, 3, \ldots, n\}$. However, due to the symmetry $k \longleftrightarrow n - k + 2$, one can restrict i to $\{2, 3, 4, \ldots, \lfloor n/2 \rfloor + 1\}$. Denoting the graph C_n by $C_n(k, \ell)$, where k and ℓ are the numbers of the vertices v and w, respectively. The spiro-chain of the graph $C_n(k, \ell)$ can be considered as the chain graph $C(G, G, \ldots, G; v, w, v, w, \ldots, v, w)$, where $G = C_n(k, \ell)$. The spiro-chains of C_3, C_4, C_6 are shown in Fig. 6. We denote the spiro-chain containing d times the component $C_n(k, \ell)$, by $S_d(C_n(k, \ell))$.

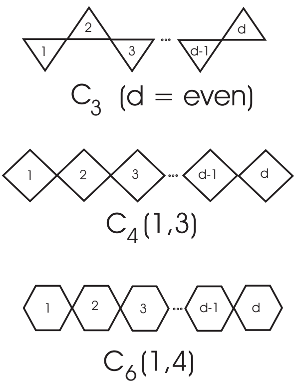

Fig. 6. The spiro-chains of C_3, C_4, and C_6.

Since all vertices of $C_n(k, \ell)$ are of degree two, it is $M_1(C_n(k, \ell)) = M_2(C_n(k, \ell)) = 4n$, $\nu = \omega = 2$, and $\alpha_{C_n(k,\ell)}(v) = \alpha_{C_n(k,\ell)}(w) = 4$. Application of Corollary 4.3 yields:

$$M_1(S_d(C_n(k, \ell))) = 4nd + 2(d-1) \times 4 = 4nd + 8d - 8 \ .$$

Also by Corollary 4.5,

$$\begin{aligned} M_2(S_d(C_n(1,2))) &= M_2(S_d(C_n(1,n))) \\ &= 4nd + (d-1)(2\times 4 + 2\times 4) + (d-2)\times 4 = 4nd + 20d - 24 \end{aligned}$$

and for $\ell \in \{2,3,\ldots,n-1\}$,

$$M_2(S_d(C_n(1,\ell))) = 4nd + (d-1)(2\times 4 + 2\times 4) = 4nd + 16d - 16 \ .$$

Example 5.3. Consider the bridge graph $G = B_1(C_n, C_n, \ldots, C_n; v, v, \ \ldots, v)$, ($d$ times), where v is an arbitrary vertex of the n-cycle C_n, see Fig. 7 for the case $n = 5$.

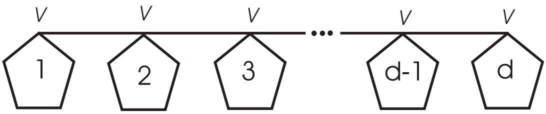

Fig. 7. The bridge graph $G = B_1(C_5, C_5, \ldots, C_5; v, v, \ldots, v)$, ($d$ times).

Application of Corollary 2.3 yields:

$$M_1(G) = 4nd + 4\times 2(d-1) + 4d - 6 = 4nd + 12d - 14 \ .$$

Similarly, using Corollary 2.5, for $d \geq 3$ we have:

$$M_2(G) = 4nd + (d-1)((2+2)^2 + 2\times 4) - 2(2+2) = 4nd + 24d - 32$$

whereas Corollary 3.5, for $d = 2$ yields:

$$M_2(G) = 2(4n) + (2-1)[(2+2) + (2\times 2) + (2+2) + (2+2) + 1] = 8n + 17 \ .$$

Example 5.4. Consider the square comb lattice graph $C_q(N)$ with open ends, where $N = n^2$ is the number of its vertices (see Fig. 8). This graph can be represented as the bridge graph $B_1(P_n, P_n, \ldots, P_n; v, v, \ldots, v)$, ($n$ times), where P_n is the path with n vertices and v is its first vertex (vertex of degree one). It is easy to see that, $M_1(P_n) = 4n - 6$ ($n \geq 2$), $M_2(P_2) = 1$, and $M_2(P_n) = 4n - 8$ ($n \geq 3$). Application of Corollary 2.3 yields:

$$M_1(C_q(N)) = n(4n-6) + 4(n-1) + 4n - 6 = 4n^2 + 2n - 10 \quad , \quad n \geq 2 \ .$$

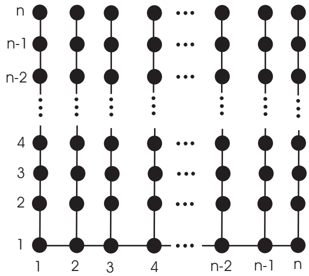

Fig. 8. The square comb lattice graph with $N = n^2$ vertices.

Similarly, using Corollary 3.5 for the case $n = 2$, and Corollary 2.5 for $n \geq 3$, we get:

$$M_2(C_q(N)) = \begin{cases} (2 \times 1) + (2-1)[1 + 1 + (1 \times 1) + 1 + 1 + 1] & \textit{if} \quad n = 2 \\ n(4n-8) + (n-1)[(1+2)^2 + 2 \times 2] - 2(1+2) & \textit{if} \quad n \geq 3 \end{cases}$$

$$= \begin{cases} 8 & \textit{if} \quad n = 2 \\ 4n^2 + 5n - 19 & \textit{if} \quad n \geq 3 \ . \end{cases}$$

Example 5.5. We consider the van Hove comb lattice graph $CvH(N)$ with open ends, where $N = n^2$ is the number of its vertices (see Fig. 9). This graph can be represented as the bridge graph

$$B_1(P_1, P_2, \ldots, P_{n-1}, P_n, P_{n-1}, \ldots, P_2, P_1; v_{1,1}, v_{1,2}, \ldots, v_{1,n-1}, v_{1,n}, v_{1,n-1}, \ldots, v_{1,2}, v_{1,1})$$

where for $2 \leq i \leq n$, $v_{1,i}$ is the first vertex (vertex of degree one) of the i-vertex path P_i and $v_{1,1}$ is the single vertex (vertex of degree zero) of singleton graph P_1 .

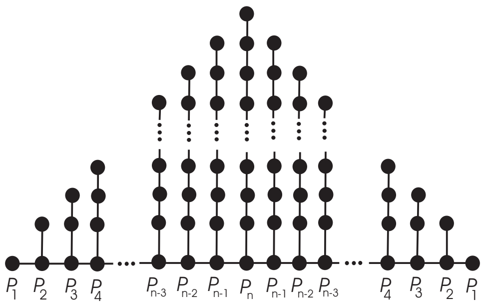

Fig. 9. The van Hove comb lattice graphs with $N = n^2$ vertices.

Clearly, $M_1(P_1) = M_2(P_1) = 0$. Application of Theorem 2.2 yields:

$$\begin{aligned} M_1(CvH(N)) &= 0 + 2\sum_{i=2}^{n-1}(4i-6) + (4n-6) + (2\times 0) \\ &+ 4\sum_{i=2}^{2n-2} 1 + (2\times 0) + 4(2n-1) - 6 = 4n^2 + 4n - 12\ . \end{aligned}$$

Similarly, using Theorem 2.4 we have for $n = 2$:

$$\begin{aligned} M_2(CvH(N)) &= (0+1+0) + 0 + 0 + 2\times 1 + (0\times 1 + 1\times 0) \\ &+ 2(0+0) - (1+1) + 4\times 1 + 4(3-2) = 9 \end{aligned}$$

whereas for $n \geq 3$,

$$\begin{aligned} M_2(CvH(N)) &= 2\left(0 + 1 + \sum_{i=3}^{n-1}(4i-8)\right) + (4n-8) + 0 + 0 \\ &+ 2\left[2\left(1 + \sum_{i=3}^{n-1} 2\right) + 2\right] + 0\times 1 + \sum_{i=2}^{2n-3} 1 + 0\times 1 \\ &+ 2(0+0) - (1+1) + 4\sum_{i=2}^{2n-2} 1 + 4(2n-1-2) \\ &= 4n^2 + 10n - 28\ . \end{aligned}$$

Example 5.6. In our last example, we consider the molecular graph of the nanostar dendrimer D_n shown in Fig. 10.

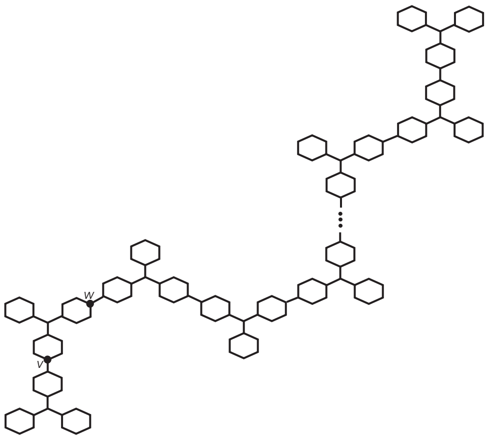

Fig. 10. The molecular graph of nanostar dendrimer D_n.

This graph can be viewed as the bridge graph $B_2(G, G, \ldots, G; v, w, v, w, \ldots, v, w)$, (n times), where G is the graph depicted in Fig. 11, v and w are the vertices shown in Fig. 10, and n is the number of repetition of the fragment G.

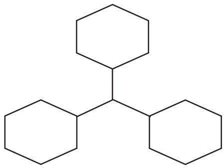

Fig. 11. The graph of nanostar dendrimer D_n for $n = 1$.

It is easy to see that $M_1(G) = 15 \times 4 + 4 \times 9 = 96$ and $M_2(G) = 12(2 \times 2) + 6(2 \times 3) + 3(3 \times 3) = 111$. Application of Corollary 3.3 yields then:

$$M_1(D_n) = 96n + 2(n-1)(2+2+1) = 106n - 10 \ .$$

Similarly, using Corollary 3.5,

$$M_2(D_n) = 111n + (n-1)[2+2+(2 \times 2)+4+4+1] = 128n - 17 \ .$$

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