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Harmonic Index of Bridge and Chain Graphs

Research Article

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Abstract: The harmonic index $H(G)$ of a graph G is defined as the sum of the weights $\dfrac{2}{d(u)+d(v)}$ of all edges uv of G, where $d(u)$ denotes the degree of the vertex u in G. In this work, we obtain harmonic index of bridge and chain graphs. Using these results, harmonic index of chemical graphs are computed.

MSC: 05C07, 05C12.

Keywords: Harmonic Index, Bridge Graph, Chain Graph.

1. Introduction

For a graph G, the harmonic index is defined as $H(G)=\sum\limits_{uv\in E(G)}\dfrac{2}{d(u)+d(v)}$ where $d(u)$ is the degree of the vertex u in G. As far as we know, this index first appeared in [9]. In 2012, Zhong reintroduced this index as harmonic index and found the minimum and maximum values of the harmonic index for simple connected graphs and trees [14]. To know more about this index refer [1–3, 6–8, 10, 12, 14–16]. Some topological indices of bridge and chain graphs have been computed, previously [4, 11, 13]. In this work, we obtain harmonic index of bridge and chain graphs. Using these results, harmonic index 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 v 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 $N_G(v)$. For other notations in graph theory, may be consulted[5].

1.1. Preliminaries

We can recall the definitions of bridge and chain graphs.

Definition 1.1. *Let $\{G_i\}_{i=1}^{k}$ be a set of finite pairwise 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 $B_1 = B_1(G_1, G_2, ..., G_k; u_1, v_1, u_2, v_2, u_3, v_3, ..., u_k, v_k)$ 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 $G_1, G_2, ..., G_k$ 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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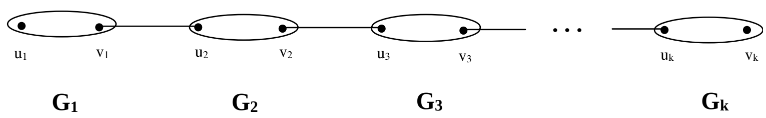

Figure 1. **The bridge graph** $B_1 = B_1(G_1, G_2, ..., G_k; u_1, v_1, u_2, v_2, ..., u_k, v_k)$

Definition 1.2. *Let* $\{G_i\}_{i=1}^k$ *be a set of finite pairwise disjoint graphs with distinct vertices* $u_i, v_i \in V(G_i)$ *such that* u_i *and* v_i *are adjacent in* G_i*. The bridge graph* $B_2 = B_2(G_1, G_2, ..., G_k; u_1, v_1, u_2, v_2, u_3, v_3, ..., u_k, v_k)$ *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* $G_1, G_2, ..., G_k$ *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 2.*

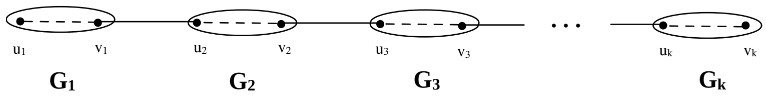

Figure 2. **The bridge graph** $B_2 = B_2(G_1, G_2, ..., G_k; u_1, v_1, u_2, v_2, ..., u_k, v_k)$

Definition 1.3. *Let* $\{G_i\}_{i=1}^k$ *be a set of finite pairwise disjoint graphs with vertices* $v_i \in V(G_i)$*. The bridge graph* $B_3 = B_3(G_1, G_2, ..., G_k; v_1, v_2, v_3, ..., v_k)$ *of* $\{G_i\}_{i=1}^k$ *with respect to the vertices* $\{v_i\}_{i=1}^k$ *is the graph obtained from 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 3.*

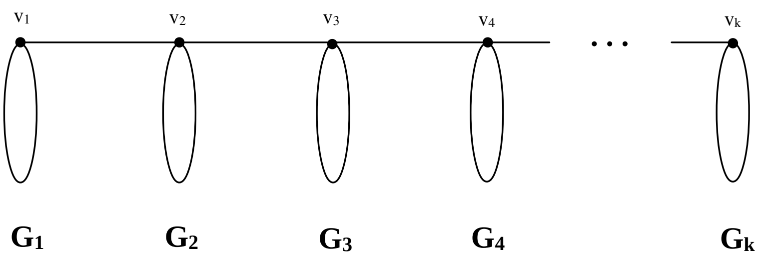

Figure 3. $B_3 = B_3(G_1, G_2, ..., G_k; v_1, v_2, v_3, ..., v_k)$

Definition 1.4. *Let* $\{G_i\}_{i=1}^k$ *be a set of finite pairwise 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 chain graph* $C_1 = C_1(G_1, G_2, ..., G_k; u_1, v_1, u_2, v_2, u_3, v_3, ..., u_k, v_k)$ *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* $G_1, G_2, ..., G_k$ *by identifying the vertices* v_i *and* u_{i+1} *for all* $i = 1, 2, ..., k-1$ *as shown in the Figure 4.*

Definition 1.5. *Let* $\{G_i\}_{i=1}^k$ *be a set of finite pairwise disjoint graphs with distinct vertices* $u_i, v_i \in V(G_i)$ *such that* u_i *and* v_i *are adjacent in* G_i*. The chain graph* $C_2 = C_2(G_1, G_2, ..., G_k; u_1, v_1, u_2, v_2, u_3, v_3, ..., u_k, v_k)$ *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* $G_1, G_2, ..., G_k$ *by identifying the vertices* v_i *and* u_{i+1} *for all* $i = 1, 2, ..., k-1$ *as shown in the Figure 5.*

2. Harmonic Index of Bridge Graphs

In this section, we compute harmonic index of three bridge graphs, namely, B_1, B_2 and B_3.

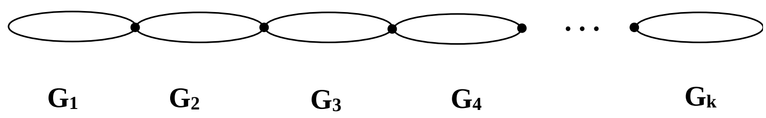

Figure 4. **The chain graph** $C_1 = C_1(G_1, G_2, ..., G_k; u_1, v_1, u_2, v_2, ..., u_k, v_k)$

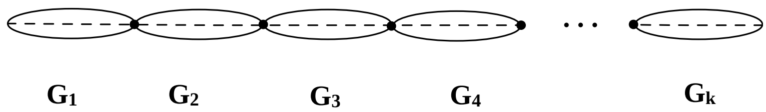

Figure 5. **The chain graph** $C_2 = C_2(G_1, G_2, ..., G_k; u_1, v_1, u_2, v_2, ..., u_k, v_k)$

Theorem 2.1. *The harmonic index of the bridge graph* $B_1, k \geq 2$ *is given by*

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

Proof. By the definition of harmonic index, $H(B_1)$ is equal to the sum of $\frac{2}{d_{B_1}(x)+d_{B_1}(y)}$, where the summation is taken over all edges $xy \in E(B_1)$. From the definition of the bridge graph B_1, $E(B_1) = E(G_1) \cup E(G_2) \cup ... \cup E(G_k) \cup \{v_i u_{i+1}; 1 \leq i \leq k-1\}$. In order to compute $H(B_1)$, we partition our sum into four sums as follows.

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

$$\begin{aligned} S_1 &= H(G_1) - \sum_{w \in N(v_1)} \frac{2}{d(v_1)+d(w)} + \sum_{w \in N(v_1)} \frac{2}{d(v_1)+d(w)+1} \\ &= H(G_1) - 2\sum_{w \in N(v_1)} \frac{1}{[d(v_1)+d(w)][d(v_1)+d(w)+1]} \end{aligned}$$

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

$$\begin{aligned} S_2 &= H(G_k) - \sum_{w \in N(u_k)} \frac{2}{d(u_k)+d(w)} + \sum_{w \in N(u_k)} \frac{2}{d(u_k)+d(w)+1} \\ &= H(G_k) - 2\sum_{w \in N(u_k)} \frac{1}{[d(u_k)+d(w)][d(u_k)+d(w)+1]} \end{aligned}$$

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

$$\begin{aligned} S_3 &= \sum_{i=2}^{k-1} H(G_i) - \sum_{i=2}^{k-1} \sum_{w \in N(u_i)} \frac{2}{[d(u_i)+d(w)]} - \sum_{i=2}^{k-1} \sum_{w \in N(v_i)} \frac{2}{[d(v_i)+d(w)]} \\ &\quad + \sum_{i=2}^{k-1} \sum_{w \in N(u_i)} \frac{2}{[d(u_i)+d(w)+1]} + \sum_{i=2}^{k-1} \sum_{w \in N(v_i)} \frac{2}{[d(v_i)+d(w)+1]} \\ &= \sum_{i=2}^{k-1} H(G_i) - 2\sum_{i=2}^{k-1} \Bigg\{ \sum_{w \in N(u_i)} \frac{1}{[d(u_i)+d(w)][d(u_i)+d(w)+1]} \\ &\quad + \sum_{w \in N(v_i)} \frac{1}{[d(v_i)+d(w)][d(v_i)+d(w)+1]} \Bigg\} \end{aligned}$$

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

$$S_4 = \sum_{i=1}^{k-1} \frac{2}{d(v_i)+d(u_{i+1})+2}$$

Now $H(B_1)$ is obtained by adding S_1, S_2, S_3, S_4. □

Suppose that u and v are two vertices of a graph G and let $G_i = G$, $v_i = v$ and $u_i = u$ for all $i = 1, 2, ..., k$.

Corollary 2.2. *If u and v are not adjacent in G, then*

$$H(B_1) = kH(G) - 2(k-1)\Big\{ \sum_{w\in N_G(u)} \frac{1}{[d(u)+d(w)][d(u)+d(w)+1]} + \sum_{w\in N_G(v)} \frac{1}{[d(v)+d(w)][d(v)+d(w)+1]} - \frac{1}{d(u)+d(v)+2} \Big\}$$

Theorem 2.3. *The harmonic index of the bridge graph $B_2, k \geq 3$ is given by*

$$\begin{aligned} H(B_2) = \sum_{i=1}^{k} H(G_i) - 2\Big\{ & \sum_{i=1}^{k-1} \sum_{w\in N(v_i)-\{u_i\}} \frac{1}{[d(v_i)+d(w)][d(v_i)+d(w)+1]} \\ & + \sum_{i=2}^{k} \sum_{w\in N(u_i)-\{v_i\}} \frac{1}{[d(u_i)+d(w)][d(u_i)+d(w)+1]} \\ & + \sum_{i=1,k} \frac{1}{[d(u_i)+d(v_i)][d(u_i)+d(v_i)+1]} \\ & + \sum_{i=2}^{k-1} \frac{2}{[d(u_i)+d(v_i)][d(u_i)+d(v_i)+2]} - \sum_{i=1}^{k-1} \frac{1}{d(v_i)+d(u_{i+1})+2} \Big\} \end{aligned}$$

Proof. By the definition of harmonic index, $H(B_2)$ 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, $E(B_2) = E(G_1) \cup E(G_2) \cup ... \cup E(G_k) \cup \{v_i u_{i+1}; 1 \leq i \leq k-1\}$. In order to compute $H(B_2)$, we partition our sum into four sums as follows.

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

$$S_1 = H(G_1) - 2 \sum_{w\in N(v_1)} \frac{1}{[d(v_1)+d(w)][d(v_1)+d(w)+1]}$$

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

$$S_2 = H(G_k) - 2 \sum_{w\in N(u_k)} \frac{1}{[d(u_k)+d(w)][d(u_k)+d(w)+1]}$$

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

$$\begin{aligned} S_3 = \sum_{i=2}^{k-1} H(G_i) - 2\sum_{i=2}^{k-1}\Big\{ & \sum_{w\in N(u_i)-\{v_i\}} \frac{1}{[d(u_i)+d(w)][d(u_i)+d(w)+1]} \\ & + \sum_{w\in N(v_i)-\{u_i\}} \frac{1}{[d(v_i)+d(w)][d(v_i)+d(w)+1]} \\ & + \frac{2}{[d(u_i)+d(v_i)][d(u_i)+d(v_i)+2]} \Big\} \end{aligned}$$

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

$$S_4 = \sum_{i=1}^{k-1} \frac{2}{d(v_i)+d(u_{i+1})+2}$$

Now $H(B_2)$ is obtained by adding S_1, S_2, S_3, S_4. □

Suppose that u and v are two vertices of a graph G and let $G_i = G$, $v_i = v$ and $u_i = u$ for all $i = 1, 2, ..., k$.

Corollary 2.4. *If u and v are adjacent in G, then*

$$H(B_2) = kH(G) - 2(k-1)\Bigg\{ \sum_{w\in N(u)-\{v\}} \frac{1}{[d(u)+d(w)][d(u)+d(w)+1]} + \sum_{w\in N(v)-\{u\}} \frac{1}{[d(v)+d(w)][d(v)+d(w)+1]} - \frac{1}{d(u)+d(v)+2}\Bigg\} - \frac{4}{d(u)+d(v)}\left[\frac{1}{d(u)+d(v)+1} + \frac{k-2}{d(u)+d(v)+2}\right]$$

Theorem 2.5. *The harmonic index of the bridge graph $B_3, k \geq 3$ is given by*

$$H(B_3) = \sum_{i=1}^{k} H(G_i) - 2\Bigg\{ \sum_{i=1,k}\sum_{w\in N(v_i)} \frac{1}{[d(v_i)+d(w)][d(v_i)+d(w)+1]} + \sum_{i=2}^{k-1}\sum_{w\in N(v_i)} \frac{2}{[d(v_i)+d(w)][d(v_i)+d(w)+2]} - \sum_{i=1,k-1} \frac{1}{[d(v_i)+d(v_{i+1})+3]} - \sum_{i=2}^{k-2} \frac{1}{[d(v_i)+d(v_{i+1})+4]}\Bigg\}$$

Proof. By the definition of harmonic index, $H(B_3)$ is equal to the sum of $\frac{2}{d_{B_3}(x)+d_{B_3}(y)}$, where the summation is taken over all edges $xy \in E(B_3)$. From the definition of the bridge graph B_3, $E(B_3) = E(G_1) \cup E(G_2) \cup ... \cup E(G_k) \cup \{v_i v_{i+1}; 1 \leq i \leq k-1\}$. In order to compute $H(B_3)$, we partition our sum into four sums as follows.

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

$$S_1 = H(G_1) - 2\sum_{w\in N(v_1)} \frac{1}{[d(v_1)+d(w)][d(v_1)+d(w)+1]}$$

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

$$S_2 = H(G_k) - 2\sum_{w\in N(v_k)} \frac{1}{[d(v_k)+d(w)][d(v_k)+d(w)+1]}$$

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

$$S_3 = \sum_{i=2}^{k-1} H(G_i) - 2\sum_{i=2}^{k-1}\sum_{w\in N(v_i)} \frac{2}{[d(v_i)+d(w)][d(v_i)+d(w)+2]}\Bigg\}$$

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

$$S_4 = \frac{2}{d(v_1)+d(v_2)+3} + \sum_{i=2}^{k-2} \frac{2}{d(v_i)+d(v_{i+1})+4} + \frac{2}{d(v_{k-1})+d(v_k)+3}$$
$$= \sum_{i=1,k-1} \frac{2}{d(v_i)+d(v_{i+1})+3} + \sum_{i=2}^{k-2} \frac{2}{d(v_i)+d(v_{i+1})+4}$$

Now $H(B_3)$ is obtained by adding S_1, S_2, S_3, S_4. □

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

Corollary 2.6. *If v is a vertex of a graph G, then*

$$H(B_3) = kH(G) - 4\Bigg\{ \sum_{w\in N(v)} \frac{1}{[d(v)+d(w)][d(v)+d(w)+1]} + (k-2)\sum_{w\in N(v)} \frac{1}{[d(v)+d(w)][d(v)+d(w)+2]} - \frac{1}{2d(v)+3} - (k-3)\frac{1}{4[d(v)+2]}\Bigg\}$$

Note that the formulae given in Theorems 2.3 and 2.5 do not hold for the case $k = 2$. Since $B_1(G_1, G_2; u_1, v_1, u_2, v_2) \equiv B_2(G_1, G_2; u_1, v_1, u_2, v_2) \equiv B_3(G_1, G_2; v_1, v_2)$, we can apply Theorem 2.1 to compute the harmonic index of bridge graphs consisting of two components.

3. Harmonic Index of Chain Graphs

In this section, we compute harmonic index of two chain graphs, namely, C_1 and C_2.

Theorem 3.1. *The harmonic index of the chain graph $C_1, k \geq 2$ is given by*

$$H(C_1) = \sum_{i=1}^{k} H(G_i) - 2\Bigg\{\sum_{i=1}^{k-1} \sum_{w\in N(v_i)} \frac{d(u_{i+1})}{[d(v_i)+d(w)][d(v_i)+d(u_{i+1})+d(w)]} + \sum_{i=2}^{k} \sum_{w\in N(u_i)} \frac{d(v_{i-1})}{[d(u_i)+d(w)][d(u_i)+d(v_{i-1})+d(w)]}\Bigg\}$$

Proof. By the definition of harmonic index, $H(C_1)$ is equal to the sum of $\frac{2}{d_{C_1}(x)+d_{C_1}(y)}$, where the summation is taken over all edges $xy \in E(C_1)$. From the definition of the bridge graph C_1, $E(C_1) = E(G_1) \cup E(G_2) \cup ... \cup E(G_k)$. In order to compute $H(C_1)$, we partition our sum into three sums as follows.

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

$$S_1 = H(G_1) - 2 \sum_{w\in N(v_1)} \frac{d(u_2)}{[d(v_1)+d(w)][d(v_1)+d(u_2)+d(w)]}$$

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

$$S_2 = H(G_k) - 2 \sum_{w\in N(u_k)} \frac{d(v_{k-1})}{[d(u_k)+d(w)][d(u_k)+d(v_{k-1})+d(w)]}$$

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

$$S_3 = \sum_{i=2}^{k-1} H(G_i) - 2\sum_{i=2}^{k-1}\Bigg\{ \sum_{w\in N(u_i)} \frac{d(v_{i-1})}{[d(u_i)+d(w)][d(u_i)+d(v_{i-1})+d(w)]} + \sum_{w\in N(v_i)} \frac{d(u_{i+1})}{[d(v_i)+d(w)][d(v_i)+d(u_{i+1})+d(w)]}\Bigg\}$$

Now $H(C_1)$ is obtained by adding S_1, S_2, S_3. □

Suppose that u and v are two vertices of a graph G and let $G_i = G$, $v_i = v$ and $u_i = u$ for all $i = 1, 2, ..., k$.

Corollary 3.2. *If u and v are not adjacent in G, then*

$$H(C_1) = kH(G) - 2(k-1)\Bigg\{ \sum_{w\in N(u)} \frac{d(v)}{[d(u)+d(w)][d(u)+d(v)+d(w)]} + \sum_{w\in N(v)} \frac{d(u)}{[d(v)+d(w)][d(v)+d(u)+d(w)]}\Bigg\}$$

Theorem 3.3. *The harmonic index of the bridge graph $C_2, k \geq 3$ is given by*

$$H(C_2) = \sum_{i=1}^{k} H(G_i) - 2\Bigg\{ \sum_{i=1}^{k-1} \sum_{w \in N(v_i)-\{u_i\}} \frac{d(u_{i+1})}{[d(v_i)+d(w)][d(v_i)+d(u_{i+1})+d(w)]}$$
$$+ \sum_{i=2}^{k} \sum_{w \in N(u_i)-\{v_i\}} \frac{d(v_{i-1})}{[d(u_i)+d(w)][d(u_i)+d(v_{i-1})+d(w)]}$$
$$+ \sum_{i=2}^{k-1} \frac{d(v_{i-1})+d(u_{i+1})}{[d(u_i)+d(v_i)][d(u_i)+d(v_{i-1})+d(v_i)+d(u_{i+1})]}$$
$$+ \frac{d(u_2)}{[d(v_1)+d(u_1)][d(v_1)+d(u_2)+d(u_1)]}$$
$$+ \frac{d(v_{k-1})}{[d(u_k)+d(v_k)][d(u_k)+d(v_{k-1})+d(v_k)]} \Bigg\}$$

Proof. By the definition of harmonic index, $H(C_2)$ is equal to the sum of $\frac{2}{d_{C_2}(x)+d_{C_2}(y)}$, where the summation is taken over all edges $xy \in E(C_2)$. From the definition of the bridge graph C_2, $E(C_2) = E(G_1) \cup E(G_2) \cup ... \cup E(G_k)$. In order to compute $H(C_2)$, we partition our sum into three sums as follows.

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

$$S_1 = H(G_1) - 2 \sum_{w \in N(v_1)} \frac{d(u_2)}{[d(v_1)+d(w)][d(v_1)+d(u_2)+d(w)]}$$

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

$$S_2 = H(G_k) - 2 \sum_{w \in N(u_k)} \frac{d(v_{k-1})}{[d(u_k)+d(w)][d(u_k)+d(v_{k-1})+d(w)]}$$

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

$$S_3 = \sum_{i=2}^{k-1} H(G_i) - \sum_{i=2}^{k-1} \sum_{w \in N(u_i)-\{v_i\}} \frac{2}{[d(u_i)+d(w)]} - \sum_{i=2}^{k-1} \sum_{w \in N(v_i)-\{u_i\}} \frac{2}{[d(v_i)+d(w)]}$$
$$- \sum_{i=2}^{k-1} \frac{2}{d(u_i)+d(v_i)} + \sum_{i=2}^{k-1} \sum_{w \in N(u_i)-\{v_i\}} \frac{2}{[d(u_i)+d(v_{i-1})+d(w)]}$$
$$+ \sum_{i=2}^{k-1} \sum_{w \in N(v_i)-\{u_i\}} \frac{2}{[d(v_i)+d(u_{i+1})+d(w)]} + \sum_{i=2}^{k-1} \frac{2}{[d(u_i)+d(v_{i-1})+d(v_i)+d(u_{i+1})]}$$
$$= \sum_{i=2}^{k-1} H(G_i) - 2 \sum_{i=2}^{k-1} \Bigg\{ \sum_{w \in N(u_i)-\{v_i\}} \frac{d(v_{i-1})}{[d(u_i)+d(w)][d(u_i)+d(v_{i-1})+d(w)]}$$
$$+ \sum_{w \in N(v_i)-\{u_i\}} \frac{d(u_{i+1})}{[d(v_i)+d(w)][d(v_i)+d(u_{i+1})+d(w)]}$$
$$+ \sum_{i=2}^{k-1} \frac{d(v_{i-1})+d(u_{i+1})}{[d(u_i)+d(v_i)][d(u_i)+d(v_{i-1})+d(v_i)+d(u_{i+1})]} \Bigg\}$$

Now $H(C_2)$ is obtained by adding S_1, S_2, S_3. □

Suppose that u and v are two vertices of a graph G and let $G_i = G$, $v_i = v$ and $u_i = u$ for all $i = 1, 2, ..., k$.

Corollary 3.4. *If u and v are adjacent in G, then*

$$H(C_2) = kH(G) - 2(k-1)\Bigg\{ \sum_{w \in N(u)-\{v\}} \frac{d(v)}{[d(u)+d(w)][d(u)+d(v)+d(w)]}$$
$$+ \sum_{w \in N(v)-\{u\}} \frac{d(u)}{[d(v)+d(w)][d(v)+d(u)+d(w)]} \Bigg\} - \frac{2}{d(u)+d(v)}$$
$$\Bigg\{ \frac{(k-2)}{2} + \frac{d(u)}{2d(u)+d(v)} + \frac{d(v)}{d(u)+2d(v)} \Bigg\}$$

Note that the formula given in Theorem 3.3 do not hold for the case $k = 2$. Since $C_1(G_1, G_2; u_1, v_1, u_2, v_2) \equiv C_2(G_1, G_2; u_1, v_1, u_2, v_2)$, we can apply Theorem 3.1 to compute the harmonic index of chain graphs consisting of two components.

4. Applications

In this section, we consider some simple molecular graphs and determine their harmonic index.

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 positions are shown in Figure 6.

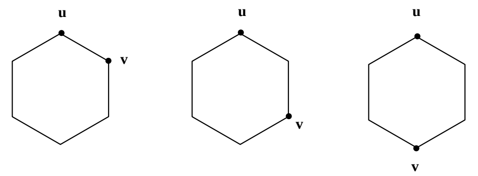

Figure 6. Ortho-, meta- and para-positions of vertices in hexagon

An internal hexagon H in a polyphenyl chain is said to be an ortho-hexagon, mete-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 7). The polyphenyl chains M_h and

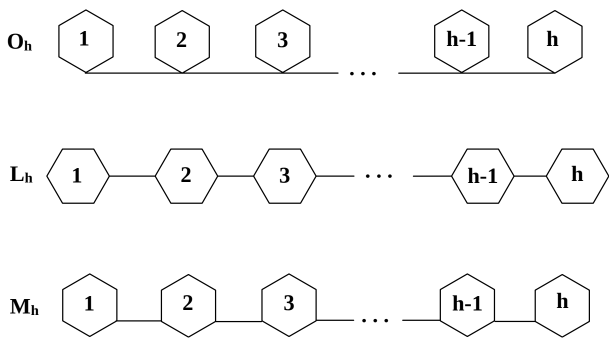

Figure 7. Ortho-, para- and meta-polyphenyl chanins with h hexagons

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 6. Since $H(C_6) = 3$, using Corollary 2.2 we obtain $H(M_h) = H(L_h) = \dfrac{44h + 1}{15}$. The polyphenyl chains O_h can be viewed as the bridge graph $B_3(C_6, C_6, ..., C_6; v, v, ..., v)(h$ times). Using Corollary 2.6, $H(O_h) = \dfrac{1225h + 37}{420}$.

Consider the square comb lattice graph $C_q(N)$ with open ends, where $N = n^2$ is the number of vertices (see Figure 8). This graph can be viewed as the bridge graph $B_3(P_n, P_n, ..., P_n; v, v, ..., v)(n$ times), where P_n is the path on n vertices and v is its first vertex. Since $H(P_n) = \frac{n}{2} - \frac{1}{6}$, by Corollary 2.6 $H(C_q(N)) = \frac{(5n-1)n}{10}$ for $n \geq 3$ and $H(C_q(N)) = \frac{11}{6}$ for $n = 2$.

Consider the spiro-chain of the cycle C_n for arbitrary $n \geq 3$. The spiro-chains of C_3, C_4, C_6 are shown in Figure 9.

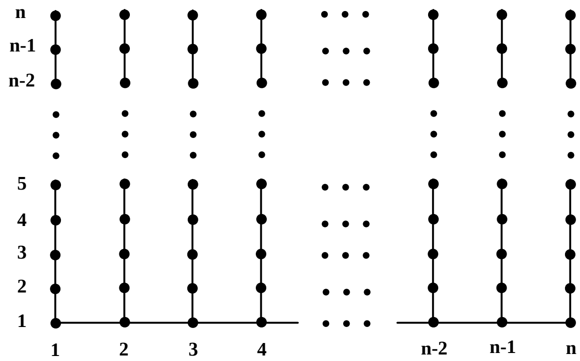

Figure 8. **The square comb lattice graph with $N = n^2$ vertices**

We denote the spiro-chain containing d times the component C_n by $S_d(C_n)$. $S_d(C_n)$ can be viewed as the chain graph

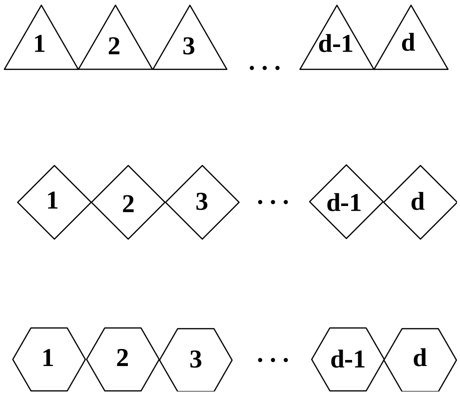

Figure 9. **The spiro-chains of C_3, C_4 and C_6**

$C_1(C_n, C_n, ..., C_n; u, v, u, v, ..., u, v)$ (d times). Since $H(C_n) = \frac{n}{2}$, by Corollary 3.2, $H(S_d(C_n)) = \frac{(3n-4)d+4}{6}; n \geq 4$. $S_d(C_3)$ can be viewed as the chain graph $C_2(C_3, C_3, ..., C_3; u, v, u, v, ..., u, v)$ (d times). Since $H(C_3) = \frac{3}{2}$, by Corollary 3.4, $H(S_d(C_3)) = \frac{11d+6}{12}$.

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