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On the Graovac–Ghorbani and Atom–Bond Connectivity Indices of Graphs from Primary Subgraphs

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ABSTRACT

Let $G = (V, E)$ be a finite simple graph. The Graovac-Ghorbani index of a graph G is defined as

$$ABC_{GG}(G) = \sum_{uv\in E(G)} \sqrt{\frac{n_u(uv,G)+n_v(uv,G)-2}{n_u(uv,G)n_v(uv,G)}},$$

where $n_u(uv, G)$ is the number of vertices closer to vertex u than vertex v of the edge $uv \in E(G)$. $n_v(uv, G)$ is defined analogously. The atom-bond connectivity index of a graph G is defined as

$$ABC(G) = \sum_{uv\in E(G)} \sqrt{\frac{d_u+d_v-2}{d_u d_v}},$$

where d_u is the degree of vertex u in G. Let G be a connected graph constructed from pairwise disjoint connected graphs $G_1, \dots, G_k$ by selecting a vertex of G_1, a vertex of G_2, and identifying these two vertices. Then continue in this manner inductively. We say that G is obtained by point-attaching from $G_1, \dots, G_k$ and that G_i's are the primary subgraphs of G. In this paper, we give some upper bounds on Graovac-Ghorbani and atom-bond connectivity indices for these graphs. Additionally, we consider some particular cases of these graphs that are of importance in chemistry and study their Graovac-Ghorbani and atom-bond connectivity indices.

1. INTRODUCTION

A molecular graph is a simple graph such that its vertices correspond to the atoms and the edges to the bonds of a molecule. Let $G = (V, E)$ be a finite, connected, simple graph. A topological index of G is a real number related to G. It does not depend on the labeling or

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pictorial representation of a graph. The Wiener index $W(G)$ is the first distance based topological index defined as $W(G) = \sum_{\{u,v\} \subseteq G} d(u,v) = \frac{1}{2}\sum_{u,v \in V(G)} d(u,v)$ with the summation runs over all pairs of vertices of G [26]. The topological indices and graph invariants based on distances between vertices of a graph are widely used for characterizing molecular graphs, establishing relationships between structure and properties of molecules, predicting biological activity of chemical compounds, and making their chemical applications. The Wiener index is one of the most used topological indices with high correlation with many physical and chemical indices of molecular compounds [26]. In 2010, Graovac et al. [14] introduced a new bond-additive structural invariant as a quantitative refinement of the distance nonbalancedness and also a measure of peripherality in graphs. They used the name Graovac-Ghorbani index for this invariant which is defined as

$$ABC_{GG}(G) = \sum_{uv \in E(G)} \sqrt{\frac{n_u(uv,G) + n_v(uv,G) - 2}{n_u(uv,G) n_v(uv,G)}},$$

where $n_u(uv,G)$ is the number of vertices of G closer to u than to v, and similarly, $n_v(uv,G)$ is the number of vertices closer to v than to u. Equidistant vertices from u and v are not taken into account to compute $n_u(uv,G)$ and $n_v(uv,G)$. They determined some bounds on this index. Graovac et al. in [15] computed that for some nanostar dendrimers. Some other upper and lower bounds on the ABC_{GG} index and also characterizing the extremal graphs was studied by Das [4]. Ghorbani et al. in [13] calculated the ABC_{GG} of an infinite family of fullerenes. More results on this index can be found in [5, 10, 20, 22, 23].

Graovac and Ghorbani defined $ABC_{GG}(G)$ [14] which motivated by the definition of atom-bond connectivity index. Initially, the atom-bond connectivity index of a graph G, $ABC(G)$, was defined [9] as:

$$ABC(G) = \sqrt{2}\sum_{uv \in E(G)} \sqrt{\frac{d_u + d_v - 2}{d_u d_v}},$$

but later on, this index was very slightly redefined [8] by dropping the factor $\sqrt{2}$. We refer the reader to [1] for a complete review of the atom-bond connectivity index.

Cactus graphs were first known as Husimi tree, they appeared in the scientific literature more than sixty years ago in papers by Husimi and Riddell concerned with cluster integrals in the theory of condensation in statistical mechanics [16, 18, 21]. We refer the reader to [2, 3, 11, 12, 17, 24, 25] for some aspects of parameters of cactus graphs.

In this paper, we consider the Graovac-Ghorbani and atom-bond connectivity indices of graphs from primary subgraphs. For convenience, the definition of these kind of graphs will be given in the next section. In Section 2, we obtain some upper bounds for Graovac-Ghorbani and atom-bond connectivity indices of graphs from primary subgraphs. In Section 3, we obtain the Graovac-Ghorbani and atom-bond connectivity indices of families of graphs that are of importance in chemistry.

2. MAIN RESULTS

Let G be a connected graph constructed from pairwise disjoint connected graphs $G_1, \dots, G_k$ as follows. Select a vertex of G_1, a vertex of G_2, and identify these two vertices. Then continue in this manner inductively. Note that the graph G constructed in this way has a tree-like structure, the G_i's being its building stones, see Figure 1.

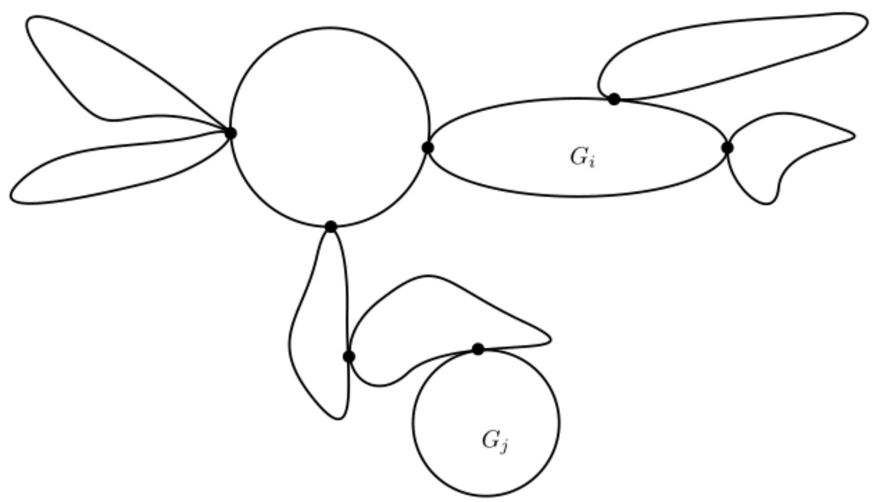

Figure 1: A graph with subgraph units $G_1, \dots, G_k$.

Usually say that G is obtained by point-attaching from $G_1, \dots, G_k$ and that G_i's are the primary subgraphs of G. A particular case of this construction is the decomposition of a connected graph into blocks (see [7]). We consider some particular cases of these graphs and study their atom-bond connectivity index. As an example of point-attaching graph, consider the graph K_m and m copies of K_n. By definition, the graph $Q(m,n)$ is obtained by identifying each vertex of K_m with a vertex of a unique K_n. The graph $Q(5,4)$ is shown in Figure 2.

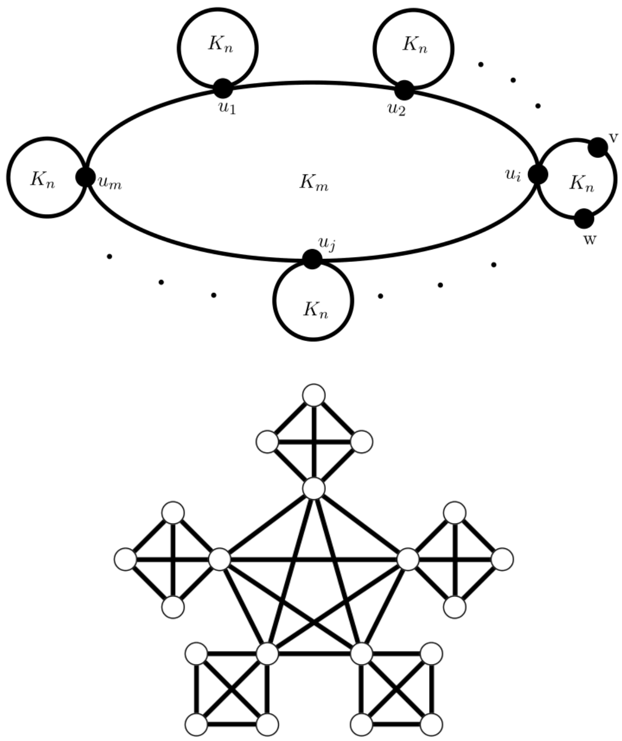

Figure 2: The graph $Q(m,n)$ and $Q(5,4)$, respectively.

Theorem 2.1. *For the graph* $Q(m,n)$ (*see Figure* 2), *and* $n \geq 2$ *we have:*

i. $$ABC(Q(m,n)) = \frac{m(m-1)}{2(m+n-2)}\sqrt{2(m+n-3)} + m\left(\frac{n}{2}-1\right)\sqrt{2(n-2)} + m(n-1)\sqrt{\frac{m+2n-5}{n^2+mn-m-3n+2}}.$$

ii. $$ABC_{GG}(Q(m,n)) = \frac{m(m-1)}{2n}\sqrt{2n-2} + m(n-1)\sqrt{\frac{n(m-1)}{n(m-1)+1}}.$$

Proof.

(i) There are $\frac{m(m-1)}{2}$ edges with endpoints of degree $m+n-2$. Also there are $m(n-1)$ edges with endpoints of degree $m+n-2$ and $n-1$, and there are $m(n-1)(\frac{n}{2}-1)$ edges with endpoints of degree $n-1$. Therefore

$$ABC(Q(m,n)) = \frac{m(m-1)}{2}\sqrt{\frac{(m+n-2)+(m+n-2)-2}{(m+n-2)(m+n-2)}} + m(n-1)\sqrt{\frac{(m+n-2)+(n-1)-2}{(m+n-2)(n-1)}} + m(n-1)\left(\frac{n}{2}-1\right)\sqrt{\frac{(n-1)+(n-1)-2}{(n-1)(n-1)}},$$

and we have the result.

(ii) First consider the edge u_iu_j in K_m. There are n vertices which are closer to u_i than u_j (including u_i itself), also there are n vertices closer to u_j than u_i, and there are $\frac{m(m-1)}{2}$ edges like u_iu_j in $Q(m,n)$. Now consider the edge vw in the i-th K_n. There is one vertex which is closer to v than w and that is v itself, and visa versa. Finally, consider the edge u_iv in the i-th K_n. There are $n(m-1)+1$ vertices which are closer to u_i than v (including u_i), also there is one vertex closer to v than u_i which is v, and there are $m(n-1)$ edges like u_iv in $Q(m,n)$.

Therefore we have the result. ■

2.1 UPPER BOUNDS

By the definition of the atom-bond connectivity and Graovac-Ghorbani indices, we have the following easy result:

Proposition 2.2. *Let G be a disconnected graph with components G_1 and G_2 Then*

i. $ABC(G) = ABC(G_1) + ABC(G_2)$.

ii. $ABC_{GG}(G) = ABC_{GG}(G_1) + ABC_{GG}(G_2)$.

Now we examine the effects on $ABC(G)$ and $ABC_{GG}(G)$ when G is modified by deleting an edge or vertex of G.

Theorem 2.3. *Let $G = (V, E)$ be a graph and $e = uv \in E$ which is not a pendant edge. Also let d_u be the degree of vertex u in G, and n_u be the number of vertices of G closer to u than to v. Then,*

i. $ABC(G-e) \geq ABC(G) - \max\left\{\frac{\sqrt{2d_u-2}}{d_v}, \frac{\sqrt{2d_v-2}}{d_u}\right\}$.

ii. $ABC_{GG}(G-e) \geq ABC_{GG}(G) - \max\left\{\frac{\sqrt{2n_u-2}}{n_v}, \frac{\sqrt{2n_v-2}}{n_u}\right\}$.

Proof. First we remove edge e and find $ABC(G-e)$. For every integer $a, b \geq 2$, we have $\sqrt{\frac{a+(b-1)-2}{a(b-1)}} \geq \sqrt{\frac{a+b-2}{ab}}$. Now Obviously, by adding edge e to $G-e$ and $\sqrt{\frac{d_u+d_v-2}{d_ud_v}}$ to $ABC(G-e)$, then $ABC(G)$ is less than that or equal to it. So

$$ABC(G) \leq ABC(G-e) + \sqrt{\frac{d_u+d_v-2}{d_ud_v}}$$

$$\leq ABC(G-e) + \max\left\{\sqrt{\frac{d_u+d_u-2}{d_vd_v}}, \sqrt{\frac{d_v+d_v-2}{d_ud_u}}\right\}$$

$$= ABC(G-e) + \max\left\{\frac{\sqrt{2d_u-2}}{d_v}, \frac{\sqrt{2d_v-2}}{d_u}\right\},$$

and therefore we have the result. The proof is similar to Part (i). ■

By the same argument as the proof of Theorem 2.3, and deleting a vertex at the first step, we have:

Theorem 2.4. *Let $G=(V,E)$ be a graph and $v \in V$. Also let d_u be the degree of vertex u in G. Then,*

i. $ABC(G-v) \geq ABC(G) - \sum_{uv \in E} \max\left\{\frac{\sqrt{2d_u-2}}{d_v}, \frac{\sqrt{2d_v-2}}{d_u}\right\}$.

ii. $ABC_{GG}(G-v) \geq ABC_{GG}(G) - \sum_{uv \in E} \max\left\{\frac{\sqrt{2n_u-2}}{n_v}, \frac{\sqrt{2n_v-2}}{n_u}\right\}$.

Here we study some bounds on the atom-bond connectivity and Graovac-Ghorbani indices for links of graphs and circuits of graphs.

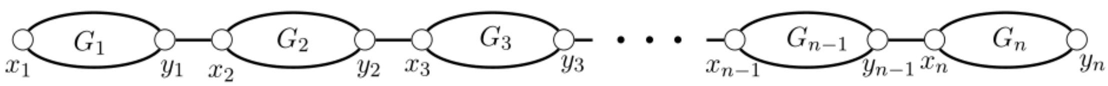

Figure 3: Link of n graphs $G_1, G_2, \dots, G_n$.

Theorem 2.5. *Let $G_1, G_2, \dots, G_k$ be a finite sequence of pairwise disjoint connected graphs and let $x_i, y_i \in V(G_i)$. Let G be the link of graphs $\{G_i\}_{i=1}^k$ with respect to the vertices $\{x_i, y_i\}_{i=1}^k$, Figure* 3, *and suppose that $G_i \neq K_1$. Then,*

i. $ABC(G) \leq \sum_{i=1}^k ABC(G_i) + \sum_{i=1}^{k-1} \max\left\{\frac{\sqrt{2d_{x_{i+1}}-2}}{d_{y_i}}, \frac{\sqrt{2d_{y_i}-2}}{d_{x_{i+1}}}\right\}$.

ii. $ABC_{GG}(G) \leq \sum_{i=1}^k ABC_{GG}(G_i) + \sum_{i=1}^{k-1} \max\left\{\frac{\sqrt{2n_{x_{i+1}}-2}}{n_{y_i}}, \frac{\sqrt{2n_{y_i}-2}}{n_{x_{i+1}}}\right\}$.

Proof. We first remove the edge y_1x_2, see Figure 3. By Theorem 2.3, we have

$$ABC(G) \leq ABC(G-y_1x_2) + \max\{\frac{\sqrt{2d_{x_2}-2}}{d_{y_1}}, \frac{\sqrt{2d_{y_1}-2}}{d_{x_2}}\}.$$

Let G' be the link graph related to graphs $\{G_i\}_{i=2}^k$ with respect to the vertices $\{x_i, y_i\}_{i=2}^k$. Then by Proposition 2.2 we have,

$$ABC(G-y_1x_2) = ABC(G_1) + ABC(G'),$$

and therefore,

$$ABC(G) \leq ABC(G_1) + ABC(G') + \max\{\frac{\sqrt{2d_{x_2}-2}}{d_{y_1}}, \frac{\sqrt{2d_{y_1}-2}}{d_{x_2}}\}.$$

By continuing this process, we have the result. The proof of (ii) is similar to Part (i). ■

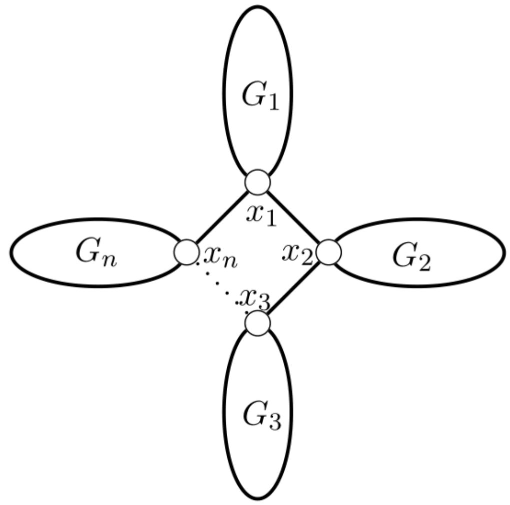

Figure 4: Circuit of n graphs $G_1, G_2, \ldots, G_n$.

Theorem 2.6. *Let $G_1, G_2, \ldots, G_k$ be a finite sequence of pairwise disjoint connected graphs and let $x_i \in V(G_i)$. Let G be the circuit of graphs $\{G_i\}_{i=1}^k$ with respect to the vertices $\{x_i\}_{i=1}^k$ and obtained by identifying the vertex x_i of the graph G_i with the i-th vertex of the cycle graph C_k (Figure 4) and suppose that $G_i \neq K_1$. Then,*

i. $$ABC(G) \leq \max\left\{\frac{\sqrt{2d_{x_1}-2}}{d_{x_n}}, \frac{\sqrt{2d_{x_n}-2}}{d_{x_1}}\right\} + \sum_{i=1}^k ABC(G_i) + \sum_{i=1}^{k-1} \max\left\{\frac{\sqrt{2d_{x_{i+1}}-2}}{d_{x_i}}, \frac{\sqrt{2d_{x_i}-2}}{d_{x_{i+1}}}\right\},$$

ii. $$ABC_{GG}(G) \leq \max\left\{\frac{\sqrt{2n_{x_1}-2}}{n_{x_n}}, \frac{\sqrt{2n_{x_n}-2}}{n_{x_1}}\right\} + \sum_{i=1}^k ABC_{GG}(G_i) + \sum_{i=1}^{k-1} \max\left\{\frac{\sqrt{2n_{x_{i+1}}-2}}{n_{x_i}}, \frac{\sqrt{2n_{x_i}-2}}{n_{x_{i+1}}}\right\}.$$

Proof. First we remove the edge $x_n x_1$, Figure 4. By Theorem 2.3, we have

$$ABC(G) \leq ABC(G - x_n x_1) + \max\{\frac{\sqrt{2d_{x_1}-2}}{d_{x_n}}, \frac{\sqrt{2d_{x_n}-2}}{d_{x_1}}\}.$$

Now we remove edge $x_1 x_2$. Then,

$$ABC(G) \leq ABC(G - \{x_n x_1, x_1 x_2\}) + \max\{\frac{\sqrt{2d_{x_1}-2}}{d_{x_n}}, \frac{\sqrt{2d_{x_n}-2}}{d_{x_1}}\} + \max\left\{\frac{\sqrt{2d_{x_2}-2}}{d_{x_1}}, \frac{\sqrt{2d_{x_1}-2}}{d_{x_2}}\right\}.$$

Let G' be the graph related to circuit graph with $\{G_i\}_{i=2}^{k}$ with respect to the vertices $\{x_i\}_{i=2}^{k}$ and removing the edge $x_n x_1$. Then by Proposition 2.2 we have,

$$ABC(G - \{x_n x_1, x_1 x_2\}) = ABC(G_1) + ABC(G'),$$

and therefore,

$$ABC(G) \leq ABC(G_1) + ABC(G') + \max\{\frac{\sqrt{2d_{x_1}-2}}{d_{x_n}}, \frac{\sqrt{2d_{x_n}-2}}{d_{x_1}}\} + \max\left\{\frac{\sqrt{2d_{x_2}-2}}{d_{x_1}}, \frac{\sqrt{2d_{x_1}-2}}{d_{x_2}}\right\}.$$

By continuing this process, we have the result. The proof of (ii) is similar to Part (i). ■

2.2 Some Other Upper Bounds for the Graovac–Ghorban Iindex

In this subsection, we consider some special graphs from primary subgraphs and present upper bounds for the Graovac-Ghorbani index of them. The following theorem is about the link of graphs.

Theorem 2.7. *Let $G_1, G_2, \ldots, G_k$ be a finite sequence of pairwise disjoint connected graphs and let $x_i, y_i \in V(G_i)$. Let G be the link of graphs $\{G_i\}_{i=1}^{k}$ with respect to the vertices $\{x_i, y_i\}_{i=1}^{k}$, see Figure* 3. *Then,*

$$ABC_{GG}(G) < (|E(G)| - (n-1)) + \sum_{i=1}^{n} ABC_{GG}(G_i) + \sum_{i=1}^{n-1} \sqrt{\frac{|V(G)|-2}{\sum_{t=1}^{i} |V(G_t)| \sum_{t=i+1}^{n} |V(G_t)|}}.$$

Proof. Consider the graph G_i (Figure 3) and let $n_{u'}(uv, G_i)$ be the number of vertices of G_i closer to u than v in G_i, Also let $n_u(uv, G_i)$ be the number of vertices of G closer to u than v in G. By the definition of Graovac-Ghorbani index, we have:

$$\begin{aligned}
ABC_{GG}(G) &= \sum_{uv \in E(G)} \sqrt{\frac{n_u(uv,G)+n_v(uv,G)-2}{n_u(uv,G)n_v(uv,G)}} \\
&= \sum_{i=1}^{n} \sum_{uv \in E(G_i)} \sqrt{\frac{n_u(uv,G_i)+n_v(uv,G_i)-2}{n_u(uv,G_i)n_v(uv,G_i)}} \\
&+ \sum_{i=1}^{n-1} \sum_{y_i x_{i+1} \in E(G)} \sqrt{\frac{n_{y_i}(y_i x_{i+1},G)+n_{x_{i+1}}(y_i x_{i+1},G)-2}{n_{y_i}(y_i x_{i+1},G)n_{x_{i+1}}(y_i x_{i+1},G)}} \\
&= \sum_{i=1}^{n} \sum_{uv \in E(G_i), d(u,x_i)<d(v,x_i), d(u,y_i)<d(v,y_i)} \sqrt{\frac{n_u(uv,G_i)+n_v(uv,G_i)-2}{n_u(uv,G_i)n_v(uv,G_i)}} \\
&+ \sum_{i=1}^{n} \sum_{uv \in E(G_i), d(u,x_i)<d(v,x_i), d(v,y_i)<d(u,y_i)} \sqrt{\frac{n_u(uv,G_i)+n_v(uv,G_i)-2}{n_u(uv,G_i)n_v(uv,G_i)}}
\end{aligned}$$

$$+\sum_{i=1}^{n}\sum_{uv\in E(G_i),d(u,x_i)<d(v,x_i),d(u,y_i)=d(v,y_i)}\sqrt{\frac{n_u(uv,G_i)+n_v(uv,G_i)-2}{n_u(uv,G_i)n_v(uv,G_i)}}$$
$$+\sum_{i=1}^{n}\sum_{uv\in E(G_i),d(u,x_i)=d(v,x_i),d(u,y_i)<d(v,y_i)}\sqrt{\frac{n_u(uv,G_i)+n_v(uv,G_i)-2}{n_u(uv,G_i)n_v(uv,G_i)}}$$
$$+\sum_{i=1}^{n}\sum_{uv\in E(G_i),d(u,x_i)=d(v,x_i),d(u,y_i)=d(v,y_i)}\sqrt{\frac{n_u(uv,G_i)+n_v(uv,G_i)-2}{n_u(uv,G_i)n_v(uv,G_i)}}$$
$$+\sum_{i=1}^{n-1}\sum_{y_ix_{i+1}\in E(G)}\sqrt{\frac{n_{y_i}(y_ix_{i+1},G)+n_{x_{i+1}}(y_ix_{i+1},G)-2}{n_{y_i}(y_ix_{i+1},G)n_{x_{i+1}}(y_ix_{i+1},G)}}$$
$$=\sum_{i=1}^{n}\sum_{uv\in E(G_i),d(u,x_i)<d(v,x_i),d(u,y_i)<d(v,y_i)}\sqrt{\frac{n_{u'}(uv,G_i)+V(G)-V(G_i)+n_{v'}(uv,G_i)-2}{(n_{u'}(uv,G_i)+V(G)-V(G_i))n_{v'}(uv,G_i)}}$$
$$+\sum_{i=1}^{n}\sum_{uv\in E(G_i),d(u,x_i)<d(v,x_i),d(v,y_i)<d(u,y_i)}\sqrt{\frac{n_{u'}(uv,G_i)+\sum_{t=1}^{i}|V(G_t)|+n_{v'}(uv,G_i)+\sum_{t=i+1}^{n}|V(G_t)|-2}{(n_{u'}(uv,G_i)+\sum_{t=1}^{i}|V(G_t)|)(n_{v'}(uv,G_i)-\sum_{t=i+1}^{n}|V(G_t)|)}}$$
$$+\sum_{i=1}^{n}\sum_{uv\in E(G_i),d(u,x_i)<d(v,x_i),d(u,y_i)=d(v,y_i)}\sqrt{\frac{n_{u'}(uv,G_i)+\sum_{t=1}^{i}|V(G_t)|+n_{v'}(uv,G_i)-2}{(n_{u'}(uv,G_i)+\sum_{t=1}^{i}|V(G_t)|)n_{v'}(uv,G_i)}}$$
$$+\sum_{i=1}^{n}\sum_{uv\in E(G_i),d(u,x_i)=d(v,x_i),d(u,y_i)<d(v,y_i)}\sqrt{\frac{n_{u'}(uv,G_i)+n_{v'}(uv,G_i)+\sum_{t=i+1}^{n}|V(G_t)|-2}{n_{u'}(uv,G_i)(n_{v'}(uv,G_i)+\sum_{t=i+1}^{n}|V(G_t)|)}}$$
$$+\sum_{i=1}^{n}\sum_{uv\in E(G_i),d(u,x_i)=d(v,x_i),d(u,y_i)=d(v,y_i)}\sqrt{\frac{n_{u'}(uv,G_i)+n_{v'}(uv,G_i)-2}{n_{u'}(uv,G_i)n_{v'}(uv,G_i)}}$$
$$+\sum_{i=1}^{n-1}\sqrt{\frac{\sum_{t=1}^{i}|V(G_t)|+\sum_{t=i+1}^{n}|V(G_t)|-2}{\sum_{t=1}^{i}|V(G_t)|\sum_{t=i+1}^{n}|V(G_t)|}}.$$

Since for every non negative integers a, b and c, $\sqrt{\frac{a+c+b-2}{(a+c)b}}<\sqrt{\frac{a+b-2}{ab}}+1$,

$$ABC_{GG}(G)<\sum_{i=1}^{n}\sum_{uv\in E(G_i),d(u,x_i)<d(v,x_i),d(u,y_i)<d(v,y_i)}\sqrt{\frac{n_{u'}(uv,G_i)+n_{v'}(uv,G_i)-2}{n_{u'}(uv,G_i)n_{v'}(uv,G_i)}}+1$$
$$+\sum_{i=1}^{n}\sum_{uv\in E(G_i),d(u,x_i)<d(v,x_i),d(v,y_i)<d(u,y_i)}\sqrt{\frac{n_{u'}(uv,G_i)+n_{v'}(uv,G_i)-2}{n_{u'}(uv,G_i)n_{v'}(uv,G_i)}}+1$$
$$+\sum_{i=1}^{n}\sum_{uv\in E(G_i),d(u,x_i)<d(v,x_i),d(u,y_i)=d(v,y_i)}\sqrt{\frac{n_{u'}(uv,G_i)+n_{v'}(uv,G_i)-2}{n_{u'}(uv,G_i)n_{v'}(uv,G_i)}}+1$$
$$+\sum_{i=1}^{n}\sum_{uv\in E(G_i),d(u,x_i)=d(v,x_i),d(u,y_i)<d(v,y_i)}\sqrt{\frac{n_{u'}(uv,G_i)+n_{v'}(uv,G_i)-2}{n_{u'}(uv,G_i)n_{v'}(uv,G_i)}}+1$$
$$+\sum_{i=1}^{n}\sum_{uv\in E(G_i),d(u,x_i)=d(v,x_i),d(u,y_i)=d(v,y_i)}\sqrt{\frac{n_{u'}(uv,G_i)+n_{v'}(uv,G_i)-2}{n_{u'}(uv,G_i)n_{v'}(uv,G_i)}}+1$$
$$+\sum_{i=1}^{n-1}\sqrt{\frac{\sum_{t=1}^{i}|V(G_t)|+\sum_{t=i+1}^{n}|V(G_t)|-2}{\sum_{t=1}^{i}|V(G_t)|\sum_{t=i+1}^{n}|V(G_t)|}}$$
$$=(|E(G)|-(n-1))+\sum_{i=1}^{n}ABC_{GG}(G_i)$$
$$+\sum_{i=1}^{n-1}\sqrt{\frac{\sum_{t=1}^{i}|V(G_t)|+\sum_{t=i+1}^{n}|V(G_t)|-2}{\sum_{t=1}^{i}|V(G_t)|\sum_{t=i+1}^{n}|V(G_t)|}},$$

and therefore we have the result. ■

By the same argument similar to the proof of the Theorem 2.7, we have the following theorem which is about the chain of graphs:

Theorem 2.8. *Let* $G_1, G_2, \ldots, G_n$ *be a finite sequence of pairwise disjoint connected graphs and let* $x_i, y_i \in V(G_i)$. *Let* $C(G_1, \ldots, G_n)$ *be the chain of graphs* $\{G_i\}_{i=1}^n$ *with respect to the vertices* $\{x_i, y_i\}_{i=1}^k$ *which obtained by identifying the vertex* y_i *with the vertex* x_{i+1} *for* $i = 1,2,\ldots, n-1$ (*Figure* 5). *Then,*

$$ABC_{GG}(C(G_1,\ldots,G_n)) < |E(G)| + \sum_{i=1}^n ABC_{GG}(G_i) + \sum_{i=1}^{n-1} \sqrt{\frac{|V(G)|-2}{\sum_{t=1}^i |V(G_t)| \sum_{t=i+1}^n |V(G_t)|}}.$$

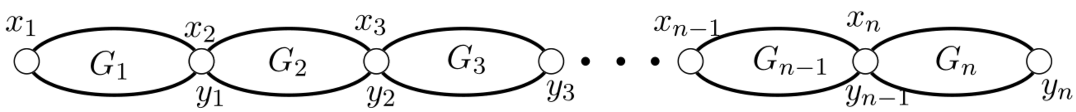

Figure 5: Chain of n graphs $G_1, G_2, \ldots, G_n$.

With similar argument to the proof of the Theorem 2.7, we have the following theorem which is about the bouquet of graphs:

Theorem 2.9. *Let* $G_1, G_2, \ldots, G_n$ *be a finite sequence of pairwise disjoint connected graphs and let* $x_i \in V(G_i)$. *Let* $B(G_1, \ldots, G_n)$ *be the bouquet of graphs* $\{G_i\}_{i=1}^n$ *with respect to the vertices* $\{x_i\}_{i=1}^n$ *and obtained by identifying the vertex* x_i *of the graph* G_i *with* x (*see Figure* 6). *Then,*

$$ABC_{GG}(B(G_1,\ldots,G_n)) < |E(G)| + \sum_{i=1}^n ABC_{GG}(G_i) + \sum_{i=1}^{n-1} \sqrt{\frac{|V(G)|-2}{\sum_{t=1}^i |V(G_t)| \sum_{t=i+1}^n |V(G_t)|}}.$$

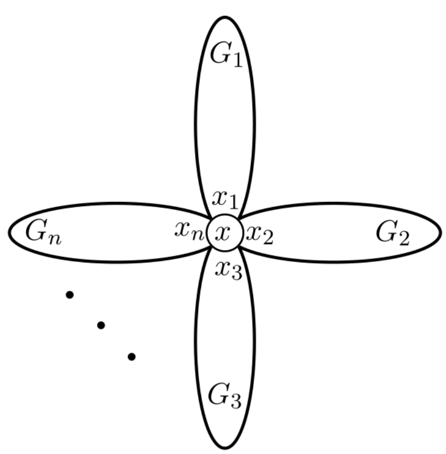

Figure 6: Bouquet of n graphs $G_1, G_2, \ldots, G_n$ and $x_1 = x_2 = \cdots = x_n = x$.

Now we consider the circuit of graphs.

Theorem 2.10. *Let $G_1, G_2, \dots, G_n$ be a finite sequence of pairwise disjoint connected graphs and let $x_i \in V(G_i)$. Let G be the circuit of graphs $\{G_i\}_{i=1}^n$ with respect to the vertices $\{x_i\}_{i=1}^n$ and obtained by identifying the vertex x_i of the graph G_i with the i-th vertex of the cycle graph C_n, Figure 4. Then,*

$$ABC_{GG}(G) < (|E(G)| - n) + \sum_{i=1}^n ABC_{GG}(G_i) + \sqrt{\frac{|V(G)|-2}{|V(G_1)||V(G_n)|}} + \sum_{i=1}^{n-1} \sqrt{\frac{|V(G)|-2}{|V(G_i)||V(G_{i+1})|}}.$$

Proof. First consider the edge x_1x_n. There are two cases, n is even or odd. If $n = 2t$ for some $t \in \mathbb{N}$, then, the vertices in the graphs $G_1, G_2, G_3, \dots, G_t$ are closer to x_1 than x_n, and the rest are closer to x_n than x_1. So,

$$\begin{aligned}\sqrt{\frac{n_{x_1}(x_1x_n,G)+n_{x_n}(x_1x_n,G)-2}{n_{x_1}(x_1x_n,G)n_{x_n}(x_1x_n,G)}} &= \sqrt{\frac{\sum_{i=1}^t |V(G_i)|+\sum_{i=1}^t |V(G_{t+i})|-2}{\sum_{i=1}^t |V(G_i)| \sum_{i=1}^t |V(G_{t+i})|}} \\ &= \sqrt{\frac{|V(G)|-2}{\sum_{i=1}^t |V(G_i)| \sum_{i=1}^t |V(G_{t+i})|}} \\ &< \sqrt{\frac{|V(G)|-2}{|V(G_1)||V(G_{2t})|}} \\ &= \sqrt{\frac{|V(G)|-2}{|V(G_1)||V(G_n)|}}.\end{aligned}$$

By the same argument, for every x_ix_{i+1}, $1 \le i \le n-1$, we have:

$$\sqrt{\frac{n_{x_i}(x_ix_{i+1},G)+n_{x_{i+1}}(x_ix_{i+1},G)-2}{n_{x_i}(x_ix_{i+1},G)n_{x_{i+1}}(x_ix_{i+1},G)}} < \sqrt{\frac{|V(G)|-2}{|V(G_i)||V(G_{i+1})|}}.$$

If $n = 2t-1$ for some $t \in \mathbb{N}$, then, the vertices in the graphs $G_1, G_2, G_3, \dots, G_{t-1}$ are closer to x_1 than x_n, and the vertices in the graphs $G_{t+1}, G_{t+2}, G_{t+3}, \dots, G_n$ are closer to x_n than x_1. The vertices in the graph G_t have the same distance to x_1 and x_n. So

$$\begin{aligned}\sqrt{\frac{n_{x_1}(x_1x_n,G)+n_{x_n}(x_1x_n,G)-2}{n_{x_1}(x_1x_n,G)n_{x_n}(x_1x_n,G)}} &= \sqrt{\frac{\sum_{i=1}^{t-1} |V(G_i)|+\sum_{i=1}^{t-1} |V(G_{t+i})|-2}{\sum_{i=1}^{t-1} |V(G_i)| \sum_{i=1}^{t-1} |V(G_{t+i})|}} \\ &= \sqrt{\frac{|V(G)|-|V(G_t)|-2}{\sum_{i=1}^{t-1} |V(G_i)| \sum_{i=1}^{t-1} |V(G_{t+i})|}}.\end{aligned}$$

Therefore,

$$\begin{aligned}\sqrt{\frac{n_{x_1}(x_1x_n,G)+n_{x_n}(x_1x_n,G)-2}{n_{x_1}(x_1x_n,G)n_{x_n}(x_1x_n,G)}} &< \sqrt{\frac{|V(G)|-|V(G_t)|-2}{|V(G_1)||V(G_{2t-1})|}} \\ &= \sqrt{\frac{|V(G)|-|V(G_t)|-2}{|V(G_1)||V(G_n)|}} \\ &< \sqrt{\frac{|V(G)|-2}{|V(G_1)||V(G_n)|}}.\end{aligned}$$

By the same argument, for every x_ix_{i+1}, $1 \le i \le n-1$, we have:

$$\sqrt{\frac{n_{x_i}(x_i x_{i+1},G)+n_{x_{i+1}}(x_i x_{i+1},G)-2}{n_{x_i}(x_i x_{i+1},G)n_{x_{i+1}}(x_i x_{i+1},G)}} < \sqrt{\frac{|V(G)|-2}{|V(G_i)||V(G_{i+1})|}}.$$

Now by the definition of Graovac-Ghorbani index and similar argument like the proof of the Theorem 2.7, we have the result. ■

3. CHEMICAL APPLICATIONS

In this section, we apply our previous results in order to obtain the atom-bond connectivity and Graovac-Ghorbani indices of families of graphs that are of importance in chemistry.

3.1 SPIRO-CHAINS

Spiro-chains are defined in [6]. Making use of the concept of chain of graphs, a spiro-chain can be defined as a chain of cycles. We denote by $S_{q,h,k}$ the chain of k cycles C_q in which the distance between two consecutive contact vertices is h, see $S_{6,2,8}$ in Figure 7.

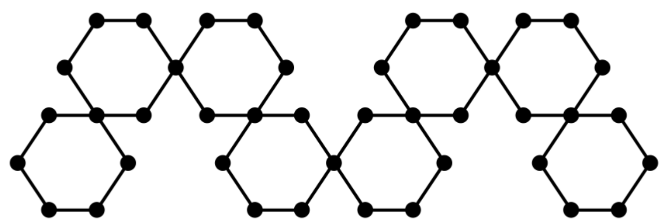

Figure 7: The graph $S_{6,2,8}$.

Theorem 3.1. *For the graph $S_{q,h,k}$ ($h \geq 2$), we have* $ABC(S_{q,h,k}) = \frac{qk}{\sqrt{2}}$.

Proof. There are $4(k-1)$ edges with endpoints of degree 2 and 4. Also there are $qk - 4(k-1)$ edges with endpoints of degree 2. Therefore

$$ABC(S_{q,h,k}) = 4(k-1)\sqrt{\frac{2+4-2}{2(4)}} + (qk-4(k-1))\sqrt{\frac{2+2-2}{2(2)}},$$

and we have the result. ■

Theorem 3.2. *For the graph $S_{q,1,k}$, we have* $ABC(S_{q,1,k}) = \frac{qk-k+2}{\sqrt{2}} + \frac{(k-2)\sqrt{6}}{4}$.

Proof. There are $k-2$ edges with endpoints of degree 4. Also there are $2k$ edges with endpoints of degree 4 and 2, and there are $qk - 3k + 2$ edges with endpoints of degree 2. Therefore by the definition of the atom-bond connectivity, we have the result. ■

Theorem 3.3. *Let T_n be the chain triangular graph of order n. Then,*

i. for every $n \geq 2$, and $k \geq 1$, if $n = 2k$, we have:

$$ABC_{GG}(T_n) = 2\sum_{i=1}^{k}\left(\sqrt{\frac{2i-2}{2i-1}} + \sqrt{\frac{4k-2i}{4k-2i+1}} + \sqrt{\frac{4k-2}{(4k-2i+1)(2i-1)}}\right),$$

and if $n = 2k+1$, thenwe have:

$$ABC_{GG}(T_n) = 2\sum_{i=1}^{k}\left(\sqrt{\frac{2i-2}{2i-1}} + \sqrt{\frac{4k-2i+2}{4k-2i+3}} + \sqrt{\frac{4k}{(4k-2i+3)(2i-1)}}\right) + 2\sqrt{\frac{2k}{2k+1}} + \frac{2\sqrt{k}}{2k+1}.$$

ii. for every $n \geq 2$, $ABC(T_n) = \frac{2n+2}{\sqrt{2}} + \frac{(n-2)\sqrt{6}}{4}$.

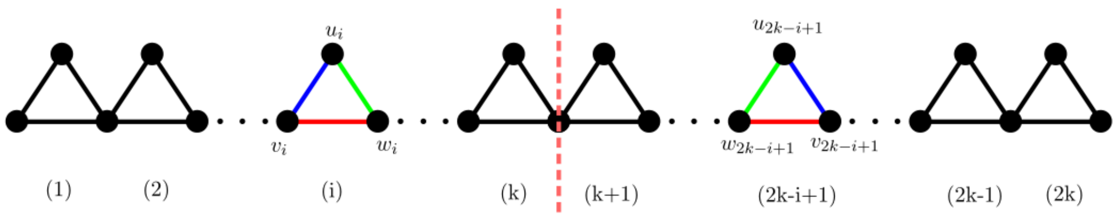

Figure 8: Chain triangular cactus T_{2k}.

Proof. (i) We consider the following cases:

Case 1. Suppose that n is even, and $n = 2k$ for some $k \in \mathbb{N}$. Consider the T_{2k} as shown in Figure 8. One can easily check that whatever happens to computation of Graovac-Ghorbani index related to the edge u_iv_i in the (i)-th triangle in T_{2k}, is the same as computation of Graovac-Ghorbani index related to the edge $u_{2k-i+1}v_{2k-i+1}$ in the $(2k-i+1)$-th triangle. The same goes for w_iv_i and $w_{2k-i+1}v_{2k-i+1}$, and also for w_iu_i and $w_{2k-i+1}u_{2k-i+1}$. So for computing Graovac-Ghorbani index, it suffices to compute the $\sqrt{\frac{n_u(uv,T_{2k})+n_v(uv,T_{2k})-2}{n_u(uv,T_{2k})n_v(uv,T_{2k})}}$ for every $uv \in E(T_{2k})$ in the first k triangles and then multiple that by 2. So from now, we only consider the first k triangles.

Consider the blue edge u_iv_i in the (i)-th triangle. There are $2(i-1)+1$ vertices which are closer to v_i than u_i, and there is one vertex closer to u_i than v_i. So, $\sqrt{\frac{n_{u_i}(u_iv_i,T_{2k})+n_{v_i}(u_iv_i,T_{2k})-2}{n_{u_i}(u_iv_i,T_{2k})n_{v_i}(u_iv_i,T_{2k})}} = \sqrt{\frac{2i-2}{2i-1}}$.

Now consider the green edge u_iw_i in the (i)-th triangle. There are $2(2k-i)+1$ vertices which are closer to w_i than u_i, and there is one vertex closer to u_i than w_i. So, $\sqrt{\frac{n_{u_i}(u_iw_i,T_{2k})+n_{w_i}(u_iw_i,T_{2k})-2}{n_{u_i}(u_iw_i,T_{2k})n_{w_i}(u_iw_i,T_{2k})}}=\sqrt{\frac{4k-2i}{4k-2i+1}}$.

Finally, consider the red edge v_iw_i in the (i)-th triangle. There are $2(2k-i)+1$ vertices which are closer to w_i than v_i, and there are $2(i-1)+1$ vertices closer to v_i than w_i. So, $\sqrt{\frac{n_{v_i}(v_iw_i,T_{2k})+n_{w_i}(v_iw_i,T_{2k})-2}{n_{v_i}(v_iw_i,T_{2k})n_{w_i}(v_iw_i,T_{2k})}}=\sqrt{\frac{4k-2}{(4k-2i+1)(2i-1)}}$.

Since we have k edges like blue one, k edges like green one and k edges like red one, by our argument, we have:

$$ABC_{GG}(T_{2k})=2\sum_{i=1}^{k}\left(\sqrt{\frac{2i-2}{2i-1}}+\sqrt{\frac{4k-2i}{4k-2i+1}}+\sqrt{\frac{4k-2}{(4k-2i+1)(2i-1)}}\right).$$

Case 2. Suppose that n is odd and $n=2k+1$ for some $k\in\mathbb{N}$. Now consider the T_{2k+1} as shown in Figure 9. One can easily check that whatever happens to computation of Graovac-Ghorbani index related to the edge u_iv_i in the (i)-th triangle in T_{2k+1}, is the same as computation of Graovac-Ghorbani index related to the edge $u_{2k-i+2}v_{2k-i+2}$ in the $(2k-i+2)$-th triangle. The same goes for w_iv_i and $w_{2k-i+2}v_{2k-i+2}$, and also for w_iu_i and $w_{2k-i+2}u_{2k-i+2}$. So for computing Graovac-Ghorbani index, it suffices to compute $\sqrt{\frac{n_u(uv,T_{2k+1})+n_v(uv,T_{2k+1})-2}{n_u(uv,T_{2k+1})n_v(uv,T_{2k+1})}}$ for every edge $uv\in E(T_{2k+1})$ in the first k triangles and then multiple that by 2 and add it to $\sum_{uv\in A}\sqrt{\frac{n_u(uv,T_{2k+1})+n_v(uv,T_{2k+1})-2}{n_u(uv,T_{2k+1})n_v(uv,T_{2k+1})}}$, where $A=\{ab,bc,ac\}$. So from now, we only consider the first k triangles and the middle one.

Consider the blue edge u_iv_i in the (i)-th triangle. There are $2(i-1)+1$ vertices which are closer to v_i than u_i, and there is one vertex closer to u_i than v_i. So, $\sqrt{\frac{n_{u_i}(u_iv_i,T_{2k+1})+n_{v_i}(u_iv_i,T_{2k+1})-2}{n_{u_i}(u_iv_i,T_{2k+1})n_{v_i}(u_iv_i,T_{2k+1})}}=\sqrt{\frac{2i-2}{2i-1}}$.

Now consider the green edge u_iw_i in the (i)-th triangle. There are $4k-2i+3$ vertices which are closer to w_i than u_i, and there is one vertex closer to u_i than w_i. So, $\sqrt{\frac{n_{u_i}(u_iw_i,T_{2k+1})+n_{w_i}(u_iw_i,T_{2k+1})-2}{n_{u_i}(u_iw_i,T_{2k+1})n_{w_i}(u_iw_i,T_{2k+1})}}=\sqrt{\frac{4k-2i+2}{4k-2i+3}}$.

Next consider the red edge v_iw_i in the (i)-th triangle. There are $2(2k-i+1)+1$ vertices which are closer to w_i than v_i, and there are $2(i-1)+1$ vertices closer to v_i than w_i. So , $\sqrt{\frac{n_{v_i}(v_iw_i,T_{2k+1})+n_{w_i}(v_iw_i,T_{2k+1})-2}{n_{v_i}(v_iw_i,T_{2k+1})n_{w_i}(v_iw_i,T_{2k+1})}}=\sqrt{\frac{4k}{(4k-2i+3)(2i-1)}}$.

Finally, consider the middle triangle. For the edge ab, there are $2k+1$ vertices which are closer to b than a, and there is one vertex closer to a than b. Also for the edge ac, there are $2k+1$ vertices which are closer to c than a, and there is one vertex closer to a than c and for the edge bc, there are $2k+1$ vertices which are closer to b than c, and there are $2k+1$ vertices closer to c than b. Hence, $\sum_{uv\in A}\sqrt{\frac{n_u(uv,T_{2k+1})+n_v(uv,T_{2k+1})-2}{n_u(uv,T_{2k+1})n_v(uv,T_{2k+1})}} = 2\sqrt{\frac{2k}{2k+1}} + \frac{\sqrt{4k}}{2k+1}$, where $A = \{ab, bc, ac\}$.

Since we have k edges like blue one, k edges like green one and k edges like red one, by our argument, we have:

$$ABC_{GG}(T_{2k+1}) = 2\sum_{i=1}^{k}\left(\sqrt{\frac{2i-2}{2i-1}} + \sqrt{\frac{4k-2i+2}{4k-2i+3}} + \sqrt{\frac{4k}{(4k-2i+3)(2i-1)}}\right) + 2\sqrt{\frac{2k}{2k+1}} + \frac{2\sqrt{k}}{2k+1}.$$

Therefore, we have the result.

(ii) It follows from Theorem 3.2. ■

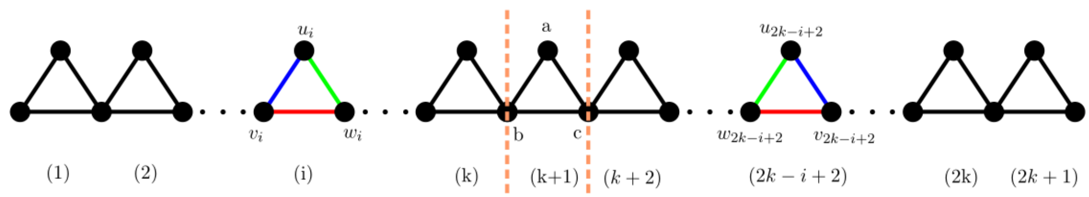

Figure 9: Chain triangular cactus T_{2k+1}.

Theorem 3.4. *.Let Q_n be the para-chain square cactus graph of order n. Then,*

i. for every $n \geq 1$, and $k \geq 1$, we have:

$$ABC_{GG}(Q_n) = \begin{cases} 8\sum_{i=1}^{k}\sqrt{\frac{6k-1}{(6k-3i+2)(3i-1)}} & if \;\; n = 2k, \\ 8\left(\sum_{i=1}^{k}\sqrt{\frac{6k+2}{(6k-3i+5)(3i-1)}}\right) + \frac{4\sqrt{6k+2}}{3k+2} & if \;\; n = 2k+1. \end{cases}$$

ii. for every $n \geq 2$, $ABC(Q_n) = 2n\sqrt{2}$.

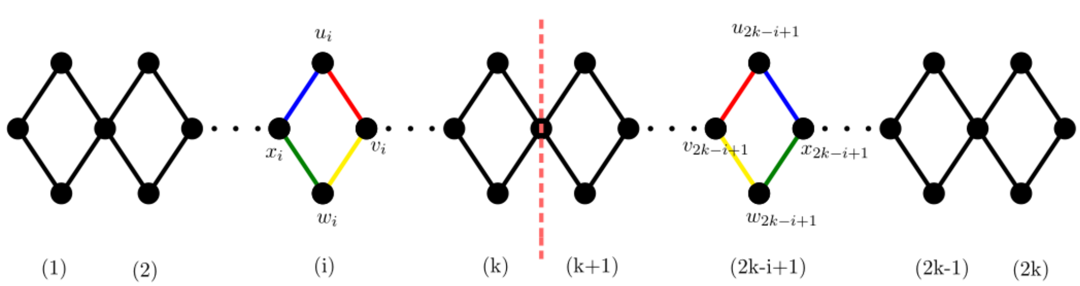

Figure 10: Para-chain square cactus Q_{2k}.

Proof. (i) We consider the following cases:

Case 1. Suppose that n is even and $n = 2k$ for some $k \in \mathbb{N}$. Now consider the Q_{2k} as shown in Figure 10. One can easily check that whatever happens to computation of Graovac-Ghorbani index related to the edge u_iv_i in the (i)-th rhombus in Q_{2k}, is the same as computation of Graovac-Ghorbani index related to the edge $u_{2k-i+1}v_{2k-i+1}$ in the $(2k-i+1)$-th rhombus. The same goes for w_iv_i and $w_{2k-i+1}v_{2k-i+1}$, for w_ix_i and $w_{2k-i+1}x_{2k-i+1}$, and also for x_iu_i and $x_{2k-i+1}u_{2k-i+1}$. So for computing Graovac-Ghorbani index, it suffices to compute the $\sqrt{\frac{n_u(uv,Q_{2k})+n_v(uv,Q_{2k})-2}{n_u(uv,Q_{2k})n_v(uv,Q_{2k})}}$ for every $uv \in E(Q_{2k})$ in the first k rhombus and then multiple that by 2. So from now, we only consider the first k rhombus.

Consider the red edge u_iv_i in the (i)-th rhombus. There are $3k+3(k-i)+2$ vertices which are closer to v_i than u_i, and there are $3i-1$ vertices closer to u_i than v_i. So, $\sqrt{\frac{n_{u_i}(u_iv_i,Q_{2k})+n_{v_i}(u_iv_i,Q_{2k})-2}{n_{u_i}(u_iv_i,Q_{2k})n_{v_i}(u_iv_i,Q_{2k})}} = \sqrt{\frac{6k-1}{(6k-3i+2)(3i-1)}}$.

One can easily check that the edges w_iv_i, w_ix_i and x_iu_i have the same attitude as u_iv_i. Since we have k edges like blue one, k edges like green one, k edges like yellow one and k edges like red one, then by our argument, we have $ABC_{GG}(Q_{2k}) = \ 2\left(4\sum_{i=1}^{k} \sqrt{\frac{6k-1}{(6k-3i+2)(3i-1)}}\right)$.

Case 2. Suppose that n is odd and $n = 2k+1$ for some $k \in \mathbb{N}$. Now consider the Q_{2k+1} as shown in Figure 11. One can easily check that whatever happens to computation of Graovac-Ghorbani index related to the edge u_iv_i in the (i)-th rhombus in Q_{2k+1}, is the same as computation of Graovac-Ghorbani index related to the edge $u_{2k-i+2}v_{2k-i+2}$ in the $(2k-i+2)$-th rhombus. The same goes for w_iv_i and $w_{2k-i+2}v_{2k-i+2}$, for w_ix_i and $w_{2k-i+2}x_{2k-i+2}$, and also for x_iu_i and $x_{2k-i+2}u_{2k-i+2}$. So for computing Graovac-Ghorbani index, it suffices to compute the $\sqrt{\frac{n_u(uv,Q_{2k+1})+n_v(uv,Q_{2k+1})-2}{n_u(uv,Q_{2k+1})n_v(uv,Q_{2k+1})}}$ for every $uv \in E(Q_{2k+1})$ in the first k rhombus and then multiple that by 2 and add it to $\sum_{uv\in A} \sqrt{\frac{n_u(uv,Q_{2k+1})+n_v(uv,Q_{2k+1})-2}{n_u(uv,Q_{2k+1})n_v(uv,Q_{2k+1})}}$, where $A = \{ab, bc, cd, da\}$. So from now, we only consider the first $k+1$ rhombus.

Consider the red edge u_iv_i in the (i)-th rhombus. There are $3(k+1)+3(k-i)+2$ vertices which are closer to v_i than u_i, and there are $3i-1$ vertices closer to u_i than v_i. So, $\sqrt{\frac{n_{u_i}(u_iv_i,Q_{2k+1})+n_{v_i}(u_iv_i,Q_{2k+1})-2}{n_{u_i}(u_iv_i,Q_{2k+1})n_{v_i}(u_iv_i,Q_{2k+1})}} = \sqrt{\frac{6k+2}{(6k-3i+5)(3i-1)}}$.

One can easily check that the edges w_iv_i, w_ix_i and x_iu_i have the same attitude as u_iv_i.

Now consider the middle rhombus. For the edge ab, there are $3k+2$ vertices which are closer to b than a, and there are $3k+2$ vertices closer to a than b. the edges bc, cd and da have the same attitude as ab. Hence, $\sum_{uv\in A}\sqrt{\frac{n_u(uv,Q_{2k+1})+n_v(uv,Q_{2k+1})-2}{n_u(uv,Q_{2k+1})n_v(uv,Q_{2k+1})}}=\frac{4\sqrt{6k+2}}{3k+2}$, where $A=\{ab,bc,cd,da\}$.

Since we have k edges like blue one, k edges like green one, k edges like yellow one and k edges like red one, then by our argument, we have:

$$ABC_{GG}(Q_{2k+1})=2\left(4\sum_{i=1}^{k}\sqrt{\frac{6k+2}{(6k-3i+5)(3i-1)}}\right)+\frac{4\sqrt{6k+2}}{3k+2}.$$

Therefore, we have the result.

(ii) It follows from Theorem 3.1. ∎

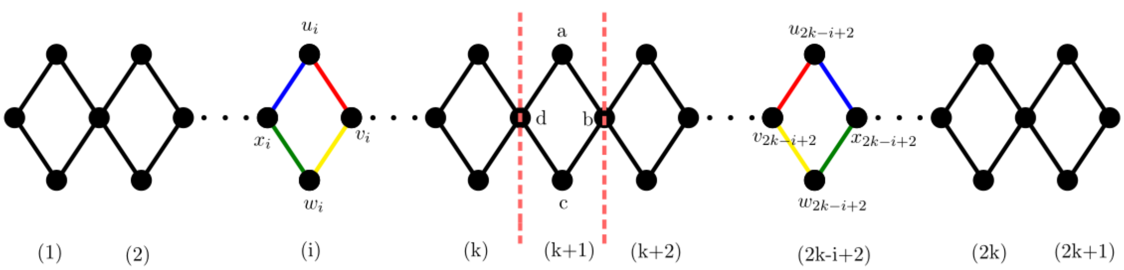

Figure 11: Para-chain square cactus Q_{2k+1}.

Theorem 3.5. *Let O_n be the para-chain square cactus graph of order n. Then,*

i. for every $n\geq 2$, and $k\geq 1$, if $n=2k$, we have:

$$ABC_{GG}(O_n)=2k\sqrt{2}+4\left(\sum_{i=1}^{k}\sqrt{\frac{6k-1}{(6k-3i+2)(3i-1)}}\right),$$

and if $n=2k+1$, thenwe have:

$$ABC_{GG}(O_n)=(2k+1)\sqrt{2}+\frac{2\sqrt{6k+2}}{3k+2}+4\left(\sum_{i=1}^{k}\sqrt{\frac{6k+2}{(6k-3i+5)(3i-1)}}\right).$$

.ii for every $n\geq 2$, $ABC(O_n)=\frac{3n+2}{\sqrt{2}}+\frac{(n-2)\sqrt{6}}{4}$.

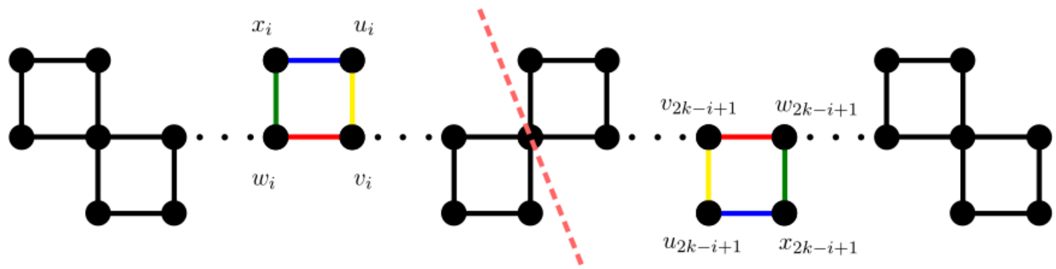

Figure 12: Para-chain square cactus O_{2k}.

Proof. (i)We consider the following cases:

Case 1. Suppose that n is even and $n = 2k$ for some $k \in \mathbb{N}$. Now consider the O_{2k} as shown in Figure 12. One can easily check that whatever happens to computation of Graovac-Ghorbani index related to the edge $u_i v_i$ in the (i)-th square in O_{2k}, is the same as computation of Graovac-Ghorbani index related to the edge $u_{2k-i+1}v_{2k-i+1}$ in the $(2k-i+1)$-th square. The same goes for $w_i v_i$ and $w_{2k-i+1}v_{2k-i+1}$, for $w_i x_i$ and $w_{2k-i+1}x_{2k-i+1}$, and also for $x_i u_i$ and $x_{2k-i+1}u_{2k-i+1}$. So for computing Graovac-Ghorbani index, it suffices to compute the $\sqrt{\frac{n_u(uv,O_{2k})+n_v(uv,O_{2k})-2}{n_u(uv,O_{2k})n_v(uv,O_{2k})}}$ for every $uv \in E(O_{2k})$ in the first k squares and then multiple that by 2. So from now, we only consider the first k squares.

Consider the yellow edge $u_i v_i$ in the (i)-th square. There are $3(2k) - 1$ vertices which are closer to v_i than u_i, and there are 2 vertices closer to u_i than v_i which is x_i. So, $\sqrt{\frac{n_{u_i}(u_i v_i,O_{2k})+n_{v_i}(u_i v_i,O_{2k})-2}{n_{u_i}(u_i v_i,O_{2k})n_{v_i}(u_i v_i,O_{2k})}} = \frac{\sqrt{2}}{2}$. By the same argument, the same happens to the edge $x_i w_i$.

Now consider the blue edge $u_i x_i$ in the (i)-th square. There are $3i - 1$ vertices which are closer to x_i than u_i, and there are $3k + 3(k - i) + 2$ vertices closer to u_i than x_i. So, $\sqrt{\frac{n_{u_i}(u_i x_i,O_{2k})+n_{x_i}(u_i x_i,O_{2k})-2}{n_{u_i}(u_i x_i,O_{2k})n_{x_i}(u_i x_i,O_{2k})}} = \sqrt{\frac{6k-1}{(6k-3i+2)(3i-1)}}$. By the same argument, the same happens to the edge $v_i w_i$.

Since we have k edges like blue one, k edges like green one, k edges like yellow one and k edges like red one, then by our argument, we have:

$$ABC_{GG}(O_{2k}) = 2\left(2\sum_{i=1}^{k}\frac{\sqrt{2}}{2} + 2\sum_{i=1}^{k}\sqrt{\frac{6k-1}{(6k-3i+2)(3i-1)}}\right).$$

Case 2. Suppose that n is odd and $n = 2k + 1$ for some $k \in \mathbb{N}$. Now consider the O_{2k+1} as shown in Figure 13. One can easily check that whatever happens to computation of Graovac-Ghorbani index related to the edge $u_i v_i$ in the (i)-th square in O_{2k+1}, is the same as computation of Graovac-Ghorbani index related to the edge $u_{2k-i+2}v_{2k-i+2}$ in the $(2k-i+2)$-th square. The same goes for w_iv_i and $w_{2k-i+2}v_{2k-i+2}$, for w_ix_i and $w_{2k-i+2}x_{2k-i+2}$, and also for x_iu_i and $x_{2k-i+2}u_{2k-i+2}$. So for computing Graovac-Ghorbani index, it suffices to compute the $\sqrt{\frac{n_u(uv,O_{2k+1})+n_v(uv,O_{2k+1})-2}{n_u(uv,O_{2k+1})n_v(uv,O_{2k+1})}}$ for every $uv \in E(O_{2k+1})$ in the first k squares and then multiple that by 2 and add it to $\sum_{uv\in A}\sqrt{\frac{n_u(uv,O_{2k+1})+n_v(uv,O_{2k+1})-2}{n_u(uv,O_{2k+1})n_v(uv,O_{2k+1})}}$, where $A=\{ab,bc,cd,da\}$. So from now, we only consider the first $k+1$ squares.

Consider the yellow edge u_iv_i in the (i)-th square. There are $3(2k+1)-1$ vertices which are closer to v_i than u_i, and there are 2 vertices closer to u_i than v_i. So, $\sqrt{\frac{n_{u_i}(u_iv_i,O_{2k+1})+n_{v_i}(u_iv_i,O_{2k+1})-2}{n_{u_i}(u_iv_i,O_{2k+1})n_{v_i}(u_iv_i,O_{2k+1})}}=\frac{\sqrt{2}}{2}$. By the same argument, the same happens to the edge x_iw_i.

Now consider the blue edge u_ix_i in the (i)-th square. There are $3i-1$ vertices which are closer to x_i than u_i, and there are $3(k+1)+3(k-i)+2$ vertices closer to u_i than x_i. So, $\sqrt{\frac{n_{u_i}(u_ix_i,O_{2k+1})+n_{x_i}(u_ix_i,O_{2k+1})-2}{n_{u_i}(u_ix_i,O_{2k+1})n_{x_i}(u_ix_i,O_{2k+1})}}=\sqrt{\frac{6k+2}{(6k-3i+5)(3i-1)}}$. By the same argument, the same happens to the edge v_iw_i.

Now consider the middle square. For the edge ab, there are $3k+2$ vertices which are closer to b than a, and there are $3k+2$ vertices closer to a than b. The edge cd has the same attitude as ab. But for the edge ad, there are $3(2k+1)-1$ vertices which are closer to d than a, and there are 2 vertices closer to a than d, and the edge bc has the same attitude as ad. Hence, $\sum_{uv\in A}\sqrt{\frac{n_u(uv,O_{2k+1})+n_v(uv,O_{2k+1})-2}{n_u(uv,O_{2k+1})n_v(uv,O_{2k+1})}}=\frac{2\sqrt{6k+2}}{3k+2}+\sqrt{2}$, where $A=\{ab,bc,cd,da\}$.

Since we have k edges like blue one, k edges like green one, k edges like yellow one and k edges like red one, then by our argument, we have:

$$ABC_{GG}(O_{2k+1})=2\left(2\sum_{i=1}^{k}\frac{\sqrt{2}}{2}+2\sum_{i=1}^{k}\sqrt{\frac{6k+2}{(6k-3i+5)(3i-1)}}\right)+\frac{2\sqrt{6k+2}}{3k+2}+\sqrt{2}.$$

Therefore, we have the result.

(ii) It follows from Theorem 3.2. ■

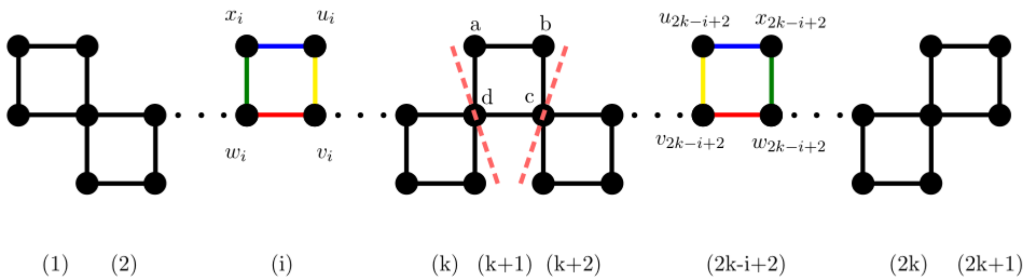

Figure 13: Para-chain square cactus O_{2k+1}.

Theorem 3.6. *Let O_n^h be the Ortho-chain graph of order n (see Figure 14). Then,*

i. for every $n \geq 2$, and $k \geq 1$, if $n = 2k$, thenwe have:

$$ABC_{GG}(O_n^h) = 4\left(\sum_{i=1}^{k} \sqrt{\frac{10k-1}{(10k-5i+3)(5i-2)}}\right) + 8k\sqrt{\frac{10k-1}{30k-6}},$$

and if $n = 2k+1$, we have:

$$ABC_{GG}(O_n^h) = 4\left(\sum_{i=1}^{k} \sqrt{\frac{10k+4}{(10k-5i+8)(5i-2)}}\right) + (8k+4)\sqrt{\frac{10k+4}{30k+9}} + \frac{2\sqrt{10k+4}}{5k+3}.$$

ii. for every $n \geq 2$, $ABC(O_n^h) = \frac{5n+2}{\sqrt{2}} + \frac{(n-2)\sqrt{6}}{4}$.

Proof. (i) It is similar to the proof of Theorem 3.5. (ii) It follows from Theorem 3.2. ■

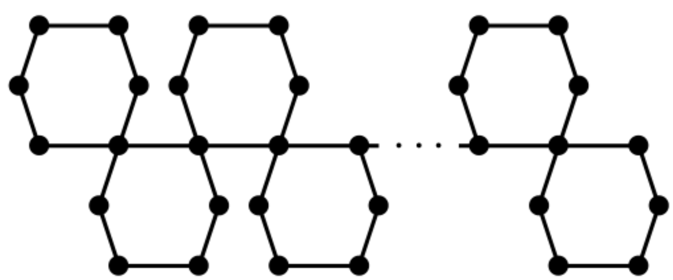

Figure 14: Ortho-chain graph O_n^h.

Theorem 3.7. *Let L_n be the para-chain hexagonal graph of order n (see Figure 15). Then,*

i. for every $n \geq 1$, and $k \geq 1$, we have:

$$ABC_{GG}(L_n) = \begin{cases} 12\sum_{i=1}^{k} \sqrt{\frac{10k-1}{(10k-5i+3)(5i-2)}} & if\ \ n = 2k, \\ 12\left(\sum_{i=1}^{k} \sqrt{\frac{10k+4}{(10k-5i+8)(5i-2)}}\right) + \frac{6\sqrt{10k+4}}{5k+3} & if\ \ n = 2k+1. \end{cases}$$

ii. for every $n \geq 2$, $ABC(L_n) = 3n\sqrt{2}$.

Proof. (i) It is similar to the proof of Theorem 3.4. (ii) It follows from Theorem 3.1. ■

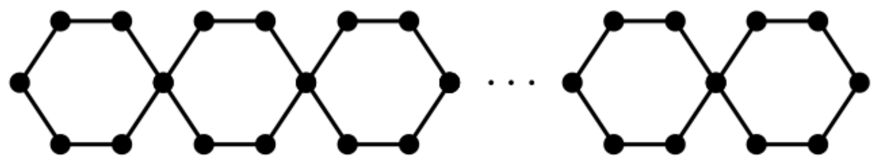

Figure 15: Para-chain hexagonal graph L_n.

Theorem 3.8. *Let M_n be the Meta-chain hexagonal of order n (see Figure 16). Then,*

i. for every $n \geq 2$, and $k \geq 1$, if $n = 2k$, we have:

$$ABC_{GG}(M_n) = 8\left(\sum_{i=1}^{k} \sqrt{\frac{10k-1}{(10k-5i+3)(5i-2)}}\right) + 4k\sqrt{\frac{10k-1}{30k-6}},$$

and if $n = 2k+1$, then we have:

$$ABC_{GG}(M_n) = 8\left(\sum_{i=1}^{k} \sqrt{\frac{10k+4}{(10k-5i+8)(5i-2)}}\right) + (2k+2)\sqrt{\frac{10k+4}{30k+9}} + \frac{4\sqrt{10k+4}}{5k+3}.$$

ii. for every $n \geq 2$, $ABC(M_n) = 3n\sqrt{2}$.

Proof. (i) It is similar to the proof of Theorem 3.5. (ii) It follows from Theorem 3.1. ■

Corollary 3.9. *Meta-chain hexagonal cactus graphs and para-chain hexagonal cactus graphs of the same order, have the same atom-bond connectivity index. But they do not have the same Graovac-Ghorbani index.*

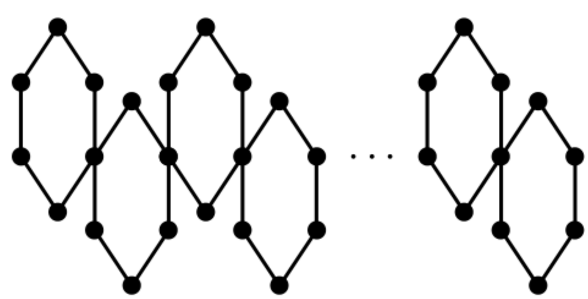

Figure 16: Meta-chain hexagonal graph M_n.

3.2 POLYPHENYLENES

Similar to the above definition of the spiro-chain $S_{q,h,k}$, we can define the graph $L_{q,h,k}$ as the link of k cycles C_q in which the distance between the two contact vertices in the same cycle is h, see $L_{6,2,4}$ in Figure 17.

Theorem 3.10. *For the graph* $L_{q,h,k}$, *when* $h \geq 2$, *we have* $ABC(L_{q,h,k}) = \frac{2(k-1)}{3} + \frac{qk}{\sqrt{2}}$.

Proof. There are $k-1$ edges with endpoints of degree 3. Also there are $4(k-1)$ edges with endpoints of degree 3 and 2, and there are $qk - 4(k-1)$ edges with endpoints of degree 2. Therefore

$$ABC(L_{q,h,k}) = (k-1)\sqrt{\frac{3+3-2}{3(3)}} + 4(k-1)\sqrt{\frac{3+2-2}{3(2)}} + (qk - 4(k-1))\sqrt{\frac{2+2-2}{2(2)}},$$

and we have the result. ■

Theorem 3.11. *For the graph* $L_{q,1,k}$, *we have:*

$$ABC(L_{q,1,k}) = \frac{4k-6}{3} + \frac{qk-k+2}{\sqrt{2}}.$$

Proof. There are $2k-3$ edges with endpoints of degree 3. Also there are $2k$ edges with endpoints of degree 3 and 2, and there are $qk - 3k + 2$ edges with endpoints of degree 2. Therefore, by the definition of the atom-bond connectivity index, we have the result. ■

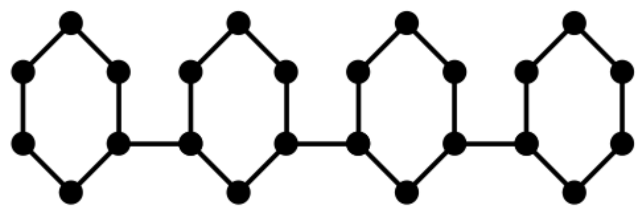

Figure 17: The graph $L_{6,2,4}$.

3.3 TRIANGULANES

We intend to derive the atom-bond connectivity of the triangulane T_k defined pictorially in [19]. We define T_k recursively in a manner that will be useful in our approach. First we define recursively an auxiliary family of triangulanes G_k $(k \geq 1)$. Let G_1 be a triangle and denote one of its vertices by y_1. We define G_k $(k \geq 2)$ as the circuit of the graphs G_{k-1}, G_{k-1}, and K_1 and denote by y_k the vertex where K_1 has been placed. The graphs G_1, G_2 and G_3 are shown in Figure 18.

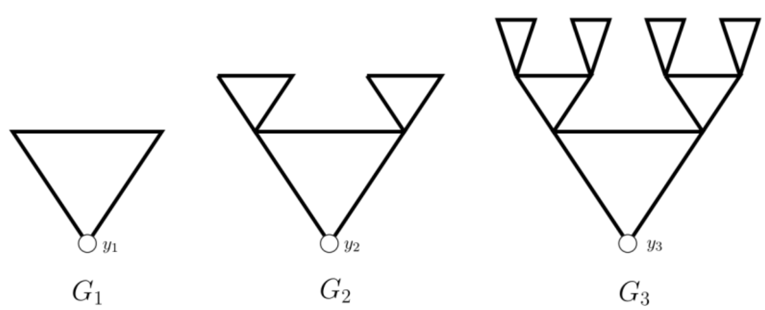

Figure 18: Graphs G_1, G_2 and G_3.

Theorem 3.12. *For the graph* T_k (*see* T_3 *in Figure* 19), *we have:*

i. $ABC(T_k) = \frac{9(2^{k-1})\sqrt{2}}{2} + \frac{(9(2^k)-6)\sqrt{6}}{4}$.

ii. $$ABC_{GG}(T_n) = 6\sqrt{\frac{2^{n+2}+2^n-4}{(2^{n+2}-1)(2^n-1)}} + \frac{3\sqrt{2^{n+2}-4}}{2^{n+1}-1}$$
$$+ \sum_{i=2}^{n} 3(2^i)\left(\sqrt{\frac{2^{n+2}+(\sum_{t=0}^{i-2} 2^{n-t})+2^{n-i+1}-4}{(2^{n+2}-1+\sum_{t=0}^{i-2} 2^{n-t})(2^{n-i+1}-1)}}\right)$$
$$+ \sum_{i=1}^{n} 3(2^{i-1})\left(\frac{\sqrt{2^{n-i+2}-4}}{2^{n-i+1}-1}\right).$$

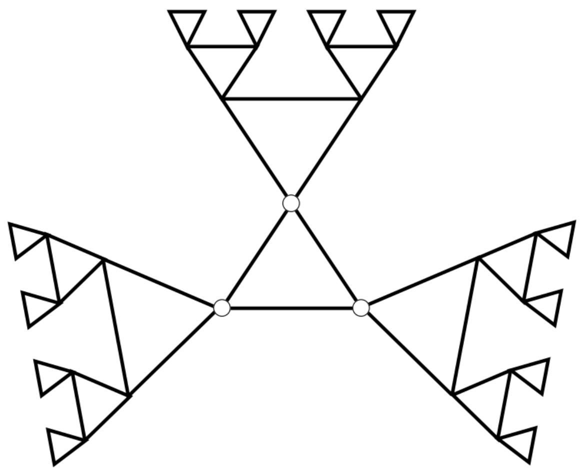

Figure 19: Graph T_3.

Proof. (i) Since creating such a graph is recursive, then there are $3 + 3\sum_{n=0}^{k-1} 3(2^n)$ edges with endpoints of degree 4. Also there are $3(2^k)$ edges with endpoints of degree 4 and 2, and there are $3(2^{k-1})$ edges with endpoints of degree 2. Therefore, by the definition of the atom-bond connectivity index, and we have the result.

(ii) Consider the graph T_n in Figure 20. First we consider the edge x_0x_1. There are $2^{n+2} - 1$ vertices which are closer to x_o than x_1, and there are $2^n - 1$ vertices closer to x_1 than x_o. So, $\sqrt{\frac{n_{x_o}(x_0x_1,T_n)+n_{x_1}(x_0x_1,T_n)-2}{n_{x_o}(x_0x_1,T_n)n_{x_1}(x_0x_1,T_n)}} = \sqrt{\frac{2^{n+2}+2^n-4}{(2^{n+2}-1)(2^n-1)}}$. The edge ax_0 has the same attitude as the blue edge x_0x_1. In total there are 6 edges with this value related to Graovac-Ghorbani index. The number of vertices closer to vertex a is the same as the number of vertices closer to vertex x_1 and are $2^n - 1$ vertices. So, $\sqrt{\frac{n_a(ax_1,T_n)+n_{x_1}(ax_1,T_n)-2}{n_a(ax_1,T_n)n_{x_1}(ax_1,T_n)}} = \frac{\sqrt{2^{n+1}-4}}{2^n-1}$, and in total, we have 3 edges like this one.

Now consider the edge x_1x_2. There are $2(2^{n+1} - 1) + 2^n + 1$ vertices which are closer to x_1 than x_2, and there are $2^{n-1} - 1$ vertices closer to x_2 than

x_1. So, $\sqrt{\frac{n_{x_o}(x_0x_1,T_n)+n_{x_1}(x_0x_1,T_n)-2}{n_{x_o}(x_0x_1,T_n)n_{x_1}(x_0x_1,T_n)}} = \sqrt{\frac{2^{n+2}+2^n+2^{n-1}-4}{(2^{n+2}+2^n-1)(2^{n-1}-1)}}$. The edge bx_1 has the same attitude as the red edge x_1x_2. In total there are 12 edges with this value related to Graovac-Ghorbani index. The number of vertices closer to vertex b is the same as the number of vertices closer to vertex x_2, and in total, and are $2^{n-1}-1$ vertices. So, $\sqrt{\frac{n_b(bx_1,T_n)+n_{x_1}(bx_1,T_n)-2}{n_b(bx_1,T_n)n_{x_1}(bx_1,T_n)}} = \frac{\sqrt{2^n-4}}{2^{n-1}-1}$, and in total, we have 6 edges like this one.

By continuing this process in the i-th level ($i > 1$), we have:

$$\sqrt{\frac{n_{x_{i-1}}(x_{i-1}x_i,T_n)+n_{x_i}(x_{i-1}x_i,T_n)-2}{n_{x_{i-1}}(x_{i-1}x_i,T_n)n_{x_i}(x_{i-1}x_i,T_n)}} = \sqrt{\frac{2^{n+2}+(\sum_{t=0}^{i-2}2^{n-t})+2^{n-i+1}-4}{(2^{n+2}-1+\sum_{t=0}^{i-2}2^{n-t})(2^{n-i+1}-1)}}.$$

We have $3(2^i)$ edges like this one. The number of vertices closer to vertex x_i is the same as the number of vertices closer to its neighbour in horizontal edge with one endpoint x_i (suppose l), and are $2^{n-i+2}-1$ vertices. So, $\sqrt{\frac{n_l(lx_1,T_n)+n_{x_1}(lx_1,T_n)-2}{n_l(lx_1,T_n)n_{x_1}(lx_1,T_n)}} = \frac{\sqrt{2^{n-i+2}-4}}{2^{n-i+1}-1}$, and in total, we have $3(2^{i-1})$ edges like this one.

Finally, the number of vertices closer to vertex x_0 is the same as the number of vertices closer to vertex u, the number of vertices closer to vertex x_0 is the same as the number of vertices closer to vertex v, and the number of vertices closer to vertex v is the same as the number of vertices closer to vertex u, and are $2^{n+1}-1$ vertices. So by the definition of the Graovac-Ghorbani index and our argument, we have

$$\begin{aligned} ABC_{GG}(T_n) &= 6\sqrt{\frac{2^{n+2}+2^n-4}{(2^{n+2}-1)(2^n-1)}} \\ &+ \sum_{i=2}^{n} 3(2^i)\left(\sqrt{\frac{2^{n+2}+(\sum_{t=0}^{i-2}2^{n-t})+2^{n-i+1}-4}{(2^{n+2}-1+\sum_{t=0}^{i-2}2^{n-t})(2^{n-i+1}-1)}}\right) \\ &+ \left(\sum_{i=1}^{n} 3(2^{i-1})\left(\frac{\sqrt{2^{n-i+2}-4}}{2^{n-i+1}-1}\right)\right) + \frac{3\sqrt{2^{n+2}-4}}{2^{n+1}-1}, \end{aligned}$$

and therefore we have the result. ■

3.4 NANOSTAR DENDRIMERS

We want to compute the atom-bond connectivity of the nanostar dendrimer D_k defined in [19]. First we define recursively an auxiliary family of rooted dendrimers G_k ($k \geq 1$). We need a fixed graph F defined in Figure 21, we consider one of its endpoint to be the root of F. The graph G_1 is defined in Figure 21, the leaf being its root. Now we define G_k ($k \geq 2$) the bouquet of the following 3 graphs: G_{k-1}, G_{k-1}, and F with respect to their roots; the root of G_k is taken to be its unique leaf (see G_2 and G_3 in Figure 22). Finally, we define D_k ($k \geq 1$) as the bouquet of 3 copies of G_k with respect to their roots (D_2 is shown in Figure 23, where the circles represent hexagons).

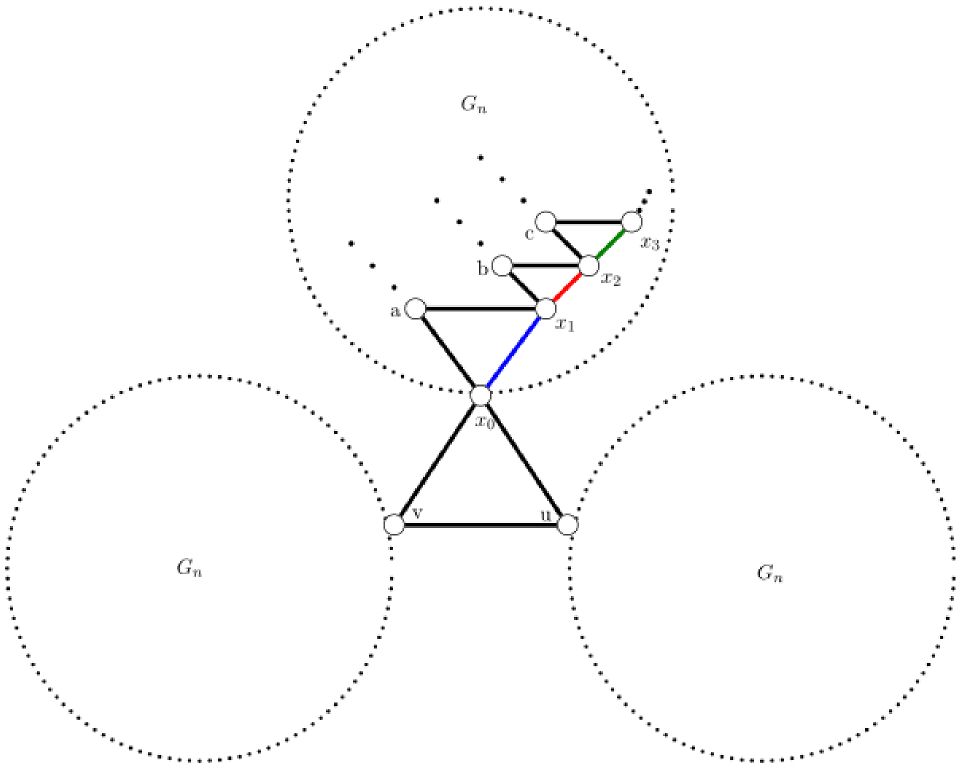

Figure 20: Graph T_n.

Figure 21: Graphs F and G_1, respectively.

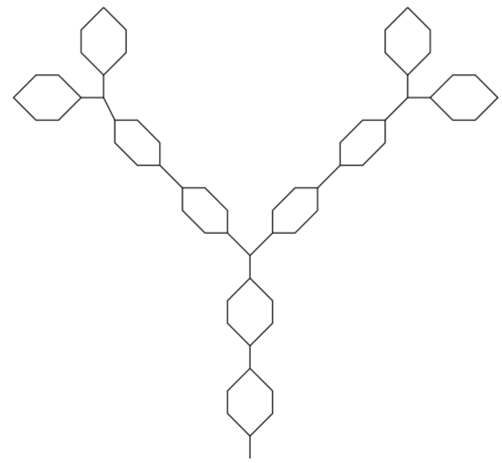

Figure 22: Graphs G_2 and G_3, respectively.

Theorem 3.13. *For the dendrimer $D_3[n]$ we have:*

$$ABC(D_3[n]) = 6(2^n) - 4 + (18(2^n) - 9)\sqrt{2}.$$

Proof. There are $3 + 9\sum_{k=0}^{n-1} 2^k$ edges with endpoints of degree 3. Also there are $6 + 18\sum_{k=0}^{n-1} 2^k$ edges with endpoints of degree 3 and 2, and there are $12 + 18\sum_{k=0}^{n-1} 2^k$ edges with endpoints of degree 2. Therefore

$$ABC(D_3[n]) = (3 + 9\sum_{k=0}^{n-1} 2^k)\sqrt{\frac{3+3-2}{3(3)}} + (6 + 18\sum_{k=0}^{n-1} 2^k)\sqrt{\frac{3+2-2}{3(2)}} + (12 + 18\sum_{k=0}^{n-1} 2^k)\sqrt{\frac{2+2-2}{2(3)}},$$

and we have the result. ■

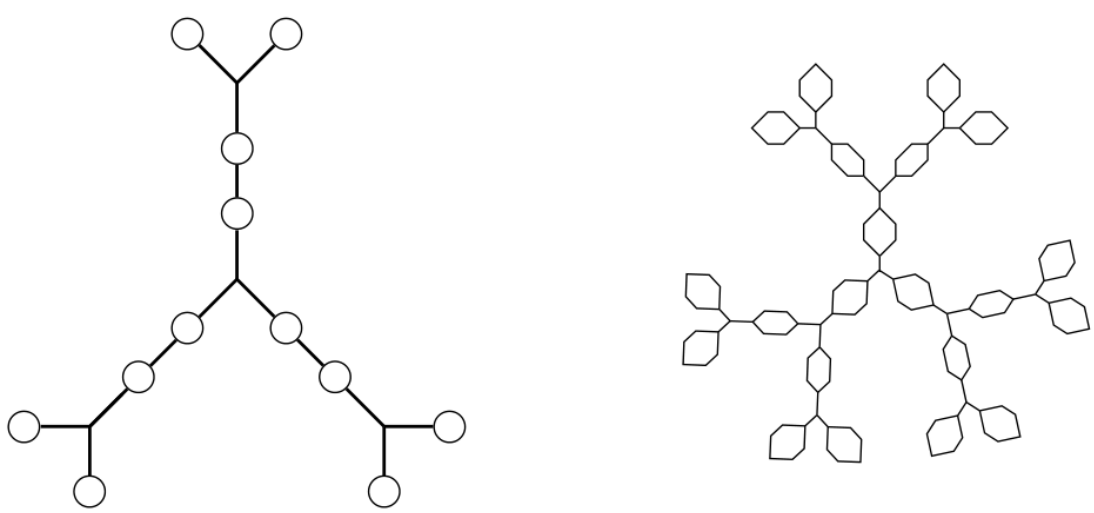

Figure 23: Nanostar D_2 and $D_3[2]$, respectively.

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