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 $ABC_{GG}(G) = \sum_{uv \in E(G)} \sqrt{n_u(uv, G) + n_v(uv, G) - 2}$, 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 $ABC(G) = \sum_{uv \in E(G)} \sqrt{d_u + d_v - 2}$, where $d_u$ is the degree of vertex $u$ in $G$. Let $G$ be a connected graph constructed from pairwise disjoint connected graphs $G_1, \ldots, G_k$ 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 $G_1, \ldots, G_k$ and that $G_i$'s are the primary subgraphs of $G$. In this paper, we give some lower and 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.

Keywords: atom-bond connectivity index, Graovac-Ghorbani index, cactus graphs.

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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 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 non-balancedness and also a measure of peripherality in graphs. They used the name Graovac-Ghorbani index for this invariant which is defined as

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

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:

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

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 lower and 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.
Figure 1: A graph with subgraph units $G_1, \ldots, G_k$.

2 Main results

Let $G$ be a connected graph constructed from pairwise disjoint connected graphs $G_1, \ldots, G_k$ 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).

Usually say that $G$ is obtained by point-attaching from $G_1, \ldots, G_k$ 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 \( m(n-1)\left(\frac{n}{2} - 1\right) \) 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. \( \square \)

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

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

Proof.

(i) 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

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

and therefore we have the result.

(ii) The proof is similar to Part (i). \qed

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

(ii) $ABC_{GG}(G - v) \geq ABC_{GG}(G) - \sum_{uv \in E} \max\{\frac{\sqrt{2n_u - 2}}{n_v}, \frac{\sqrt{2n_v - 2}}{n_u}\}$.
Here we study some bounds on the atom-bond connectivity and Graovac-Ghorbani indices for links of graphs and circuits of graphs.

**Theorem 2.5** 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) and suppose that $G_i \neq K_1$. Then,

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

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

**Proof.**

(i) First we remove edge $y_1x_2$ (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.

(ii) The proof is similar to Part (i). \qed

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

(i)

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

$$
+ \sum_{i=1}^{k-1} \max\left\{ \frac{\sqrt{2d_{x_{i+1}}}}{d_{x_i}} - \frac{2}{d_{x_1}} \right\}.
$$

(ii)

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

$$
+ \sum_{i=1}^{k-1} \max\left\{ \frac{\sqrt{2n_{x_{i+1}}}}{n_{x_i}} - \frac{2}{n_{x_1}} \right\}.
$$

Proof.

(i) First we remove edge $x_n x_1$ (Figure 4). By Theorem 2.3, we have

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

Now we remove edge $x_1 x_2$. Then,

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

$$
+ \max\left\{ \frac{\sqrt{2d_{x_1}} - 2}{d_{x_2}}, \frac{\sqrt{2d_{x_2}} - 2}{d_{x_1}} \right\}.
$$

7
Let $G'$ be the graph related to circuit graph with $\{G_i\}_{i=1}^k$ with respect to the vertices $\{x_i\}_{i=1}^k$ and removing the edge $x_nx_1$. Then by Proposition 2.2 we have,

$$ABC(G - \{x_nx_1, x_1x_2\}) = ABC(G_1) + ABC(G'),$$

and therefore,

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

By continuing this process, we have the result.

(ii) The proof is similar to Part (i). \qed

2.2 Some other Upper bounds for the Graovac-Ghorbani index

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,

$$ABC_{GG}(G) < \left( |E(G)| - (n - 1) \right) + \sum_{i=1}^{n} ABC_{GG}(G_i)$$

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

**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:

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

$$= \sum_{i=1}^{n} \sum_{uv \in E(G_i)} \sqrt{\frac{n_u(uv, G_i) + n_v(uv, G_i) - 2}{n_u(uv, G_i)n_v(uv, G_i)}}$$

$$+ \sum_{i=1}^{n-1} \sqrt{\frac{|V(G)| - 2}{\sum_{t=1}^{n} |V(G_t)| \sum_{t=i+1}^{n} |V(G_t)|}}.$$
\[ + \sum_{i=1}^{n-1} \sum_{y_i, x_{i+1} \in E(G)} \sqrt{n_{y_i}(y_i, x_{i+1}, G) + n_{x_{i+1}}(y_i, x_{i+1}, G) - 2} \]

\[ = \sum_{i=1}^{n} \sum_{u \in E(G), d(u, x_i) < d(v, x_i), d(u, y_i) < d(v, y_i)} \frac{n_{u}(uv, G_i) + n_{v}(uv, G_i) - 2}{n_{u}(uv, G_i)n_{v}(uv, G_i)} \]

\[ + \sum_{i=1}^{n} \sum_{u \in E(G), d(u, x_i) < d(v, x_i), d(u, y_i) = d(v, y_i)} \frac{n_{u}(uv, G_i) + n_{v}(uv, G_i) - 2}{n_{u}(uv, G_i)n_{v}(uv, G_i)} \]

\[ + \sum_{i=1}^{n} \sum_{u \in E(G), d(u, x_i) = d(v, x_i), d(u, y_i) = d(v, y_i)} \frac{n_{u}(uv, G_i) + n_{v}(uv, G_i) - 2}{n_{u}(uv, G_i)n_{v}(uv, G_i)} \]

\[ + \sum_{i=1}^{n-1} \sum_{y_i, x_{i+1} \in E(G)} \sqrt{n_{y_i}(y_i, x_{i+1}, G) + n_{x_{i+1}}(y_i, x_{i+1}, G) - 2} \]

\[ = \sum_{i=1}^{n} \sum_{u \in E(G), d(u, x_i) < d(v, x_i), d(u, y_i) < d(v, y_i)} \frac{n_{u}'(uv, G_i) + V(G) - V(G_i) + n_{v}'(uv, G_i) - 2}{n_{u}'(uv, G_i) + V(G) - V(G_i)n_{v}'(uv, G_i)} \]

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

\[ + \sum_{i=1}^{n} \sum_{u \in E(G), d(u, x_i) = d(v, x_i), d(u, y_i) = d(v, y_i)} \frac{n_{u}'(uv, G_i) + \sum_{t=i+1}^{n} |V(G_t)| - 2}{n_{u}'(uv, G_i)n_{v}'(uv, G_i)} \]
and therefore we have the result.

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 $\{G_i\}^n_{i=1}$ with
Figure 5: Chain of $n$ graphs $G_1, G_2, \ldots, G_n$.

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

$$ABC_{GG}(C(G_1, \ldots, G_n)) < |E(G)| + \sum_{i=1}^{n} ABC_{GG}(G_i)$$

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

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,

$$ABC_{GG}(B(G_1, \ldots, G_n)) < |E(G)| + \sum_{i=1}^{n} ABC_{GG}(G_i)$$

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

Now we consider to the circuit of graphs.
Theorem 2.10 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 $G$ 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,

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

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 $G_1, G_2, G_3, \ldots, G_t$ are closer to $x_1$ than $x_n$, and the rest are closer to $x_n$ than $x_1$. So

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

$$= \sqrt{\frac{|V(G)| - 2}{|V(G_1)||V(G_{2t})|}} < \sqrt{\frac{|V(G)| - 2}{|V(G)| - 2}}$$

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

$$\sqrt{\frac{n_{x_i}(x_ix_{i+1},G) + n_{x_{i+1}}(x_ix_{i+1},G) - 2}{n_{x_i}(x_ix_{i+1},G)n_{x_{i+1}}(x_ix_{i+1},G)}}$$

If $n = 2t - 1$ for some $t \in \mathbb{N}$, then, the vertices in the graphs $G_1, G_2, G_3, \ldots, G_{t-1}$ are closer to $x_1$ than $x_n$, and the vertices in the graphs $G_{t+1}, G_{t+2}, G_{t+3}, \ldots, G_n$ 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

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

$$= \sqrt{\frac{|V(G)| - |V(G_i)| - 2}{|V(G_i)||V(G_{t+i})|}}$$
Therefore,
\[
\sqrt{n_{x_1}(x_1x_n, G) + n_{x_n}(x_1x_n, G) - 2} < \sqrt{|V(G)| - |V(G_t)| - 2} \over |V(G_1)||V(G_{2l-1})| \]
\[
= \sqrt{|V(G)| - |V(G_t)| - 2} \over |V(G_1)||V(G_n)| \]
\[
< \sqrt{|V(G)| - 2} \over |V(G_1)||V(G_n)| \]

By the same argument, for every \(x_ix_{i+1}, 1 \leq i \leq n - 1\), we have:
\[
\sqrt{n_{x_i}(x_ix_{i+1}, G) + n_{x_{i+1}}(x_ix_{i+1}, G) - 2} < \sqrt{|V(G)| - 2} \over |V(G_i)||V(G_{i+1})| .
\]

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

\[\Box\]

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 spiro-chain \(S_{6,2,8}\) in Figure 7).

**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:

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

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

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

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

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 formula 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, 

\[
\sqrt{\frac{n_{u_i}(u_iv_i,T_{2k})+n_{w_i}(u_iv_i,T_{2k})-2}{n_{u_i}(u_iv_i,T_{2k})+n_{w_i}(u_iv_i,T_{2k})}} = \sqrt{\frac{2i-2}{2i-1}}.
\]

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, then 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.

Figure 8: Chain triangular cactus \( T_{2k} \).
triangle. The same goes for $w_iv_i$ and $w_{2k-i+1}v_{2k-i+2}$, and also for $w_iu_i$ and $w_{2k-i+1}u_{2k-i+2}$. So for computing Graovac-Ghorbani index, it suffices to compute the $\sqrt{\frac{n_u(uw,T_{2k+1})+n_v(uw,T_{2k+1})-2}{n_u(uw,T_{2k+1})n_v(uw,T_{2k+1})}}$ for every $uv \in E(T_{2k+1})$ in the first $k$ triangles and then multiply that by 2 and add it to
\[
\sum_{uv \in A} \sqrt{\frac{n_u(uw,T_{2k+1})+n_v(uw,T_{2k+1})-2}{n_u(uw,T_{2k+1})n_v(uw,T_{2k+1})}},
\]
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, $\sqrt{\frac{n_u(u_i,v_i,T_{2k+1})+n_v(u_i,v_i,T_{2k+1})-2}{n_u(u_i,v_i,T_{2k+1})n_v(u_i,v_i,T_{2k+1})}} = \sqrt{\frac{2i-2}{2i-1}}$.

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

Now consider the red edge $v_iw_i$ in the $(i)$-th triangle. There are $2(2k-1) + 1$ 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, $\sqrt{\frac{n_u(v_i,w_i,T_{2k+1})+n_v(v_i,w_i,T_{2k+1})-2}{n_u(v_i,w_i,T_{2k+1})n_v(v_i,w_i,T_{2k+1})}} = \sqrt{\frac{4k}{(4k-2i+3)(2i-1)}}$.

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, $\sum_{uv \in A} \sqrt{\frac{n_u(uw,T_{2k+1})+n_v(uw,T_{2k+1})-2}{n_u(uw,T_{2k+1})n_v(uw,T_{2k+1})}} = 2 \sqrt{\frac{2k+1 + \sqrt{4k}}{2k+1}}$, where $A = \{ab,bc,ac\}$.

Since we have $k$ edges like blue one, $k$ edges like green one and $k$ edges like red one, then 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
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:

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

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

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 the 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 $w_iu_i$ and $w_{2k-i+1}u_{2k-i+1}$, for $w_iw_{i+1}$ and $w_{2k-i+1}w_{2k-i+1}$, 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 \( \sqrt{\frac{\sum_{uv \in E(Q_{2k})} n_u(uv, Q_{2k}) + n_v(uv, Q_{2k}) - 2}{\sum_{uv \in E(Q_{2k})} n_u(uv, Q_{2k}) n_v(uv, Q_{2k})}} \) for every \( uv \in E(Q_{2k}) \) in the first \( k \) rhombus and then multiply that by 2. So from now, we only consider the first \( k \) rhombus.

Consider the red edge \( u_i v_i \) 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, \( \sqrt{\frac{\sum_{uv \in E(Q_{2k})} n_u(uv, Q_{2k}) + n_v(uv, Q_{2k}) - 2}{\sum_{uv \in E(Q_{2k})} n_u(uv, Q_{2k}) n_v(uv, Q_{2k})}} = \frac{6k-1}{(6k-3i+2)(3i-1)} \).

One can easily check that the edges \( w_i v_i \) and \( x_i u_i \) have the same attitude as \( u_i v_i \). 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 [III]. 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 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 \( w_i x_i \) and \( w_{2k-2i+2} x_{2k-2i+2} \), and also for \( x_i u_i \) and \( x_{2k-i+2} u_{2k-i+2} \).

So for computing Graovac-Ghorbani index, it suffices to compute the \( \sqrt{\frac{\sum_{uv \in E(Q_{2k+1})} n_u(uv, Q_{2k+1}) + n_v(uv, Q_{2k+1}) - 2}{\sum_{uv \in E(Q_{2k+1})} n_u(uv, Q_{2k+1}) n_v(uv, Q_{2k+1})}} \) for every \( uv \in E(Q_{2k+1}) \) in the first \( k \) rhombus and then multiple that by 2 and add it to \( \sum_{uv \in A} \sqrt{\frac{\sum_{uv \in E(Q_{2k+1})} n_u(uv, Q_{2k+1}) + n_v(uv, Q_{2k+1}) - 2}{\sum_{uv \in E(Q_{2k+1})} n_u(uv, Q_{2k+1}) n_v(uv, Q_{2k+1})}} \), where \( A = \{ab, bc, cd, da\} \). So from now, we only consider the first \( k + 1 \) rhombus.

Consider the red edge \( u_i v_i \) 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, \( \sqrt{\frac{\sum_{uv \in E(Q_{2k+1})} n_u(uv, Q_{2k+1}) + n_v(uv, Q_{2k+1}) - 2}{\sum_{uv \in E(Q_{2k+1})} n_u(uv, Q_{2k+1}) n_v(uv, Q_{2k+1})}} = \frac{6k+2}{(6k-3i+3)(3i-1)} \).

One can easily check that the edges \( w_i v_i \) and \( x_i u_i \) have the same attitude as \( u_i v_i \). 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, \( \sum_{uv \in A} \sqrt{\frac{\sum_{uv \in E(Q_{2k+1})} n_u(uv, Q_{2k+1}) + n_v(uv, Q_{2k+1}) - 2}{\sum_{uv \in E(Q_{2k+1})} n_u(uv, Q_{2k+1}) n_v(uv, Q_{2k+1})}} = 4\sqrt{\frac{6k+2}{3k+2}} \), 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:

\[
ABC_{GG}(Q_{2k+1}) = 2 \left( 4 \sum_{i=1}^{k} \sqrt{\frac{6k+2}{(6k-3i+3)(3i-1)}} \right) + 4\sqrt{\frac{6k+2}{3k+2}}.
\]
Figure 11: Para-chain square cactus $Q_{2k+1}$.

Therefore, we have the result.

(ii) It follows from Theorem 3.1.

\[\Box\]

**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:

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

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

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

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

**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 $u_iv_i$ 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 $w_iw_i$ and $w_{2k-i+1}w_{2k-i+1}$, for $x_ix_i$ and $w_{2k-i+1}x_{2k-i+1}$, and also...
Case 2. Suppose that 

Now consider the blue edge \( uv \) which are closer to \( x \). argument, the same happens to the edge \( uv \), and there are 3 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 \( u_iv_i \) 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 in-

for \( x_iu_i \) and \( x_{2k-i+1}u_{2k-i+1} \). So for computing Graovac-Ghorbani, 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 \( u_iv_i \) 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, \[
\sqrt{\frac{n_u(u_iv_i,O_{2k}) + n_v(u_iv_i,O_{2k}) - 2}{n_u(u_iv_i,O_{2k})n_v(u_iv_i,O_{2k})}} = \frac{\sqrt{2}}{2}.
\]

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 \( 3k + 3(k - i) + 2 \) vertices closer to \( u_i \) than \( x_i \). So, \[
\sqrt{\frac{n_u(u_ix_i,O_{2k}) + n_v(u_ix_i,O_{2k}) - 2}{n_u(u_ix_i,O_{2k})n_v(u_ix_i,O_{2k})}} = \sqrt{\frac{6k-1}{(6k-3i+2)(3i-1)}}.
\]

By the same argument, the same happens to the edge \( v_iw_i \).

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:
Theorem 3.6
Let $E(O_{2k+1})$ in the first $k$ squares and then multiple that by 2 and add it to $\sum_{uv \in A} \sqrt{\frac{n_u(u,v,O_{2k+1})+n_v(u,v,O_{2k+1})-2}{n_u(u,v,O_{2k+1})n_v(u,v,O_{2k+1})}}$, 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, $\sqrt{\frac{n_u(u_i,v_i,O_{2k+1})+n_v(u_i,v_i,O_{2k+1})-2}{n_u(u_i,v_i,O_{2k+1})n_v(u_i,v_i,O_{2k+1})}} = \frac{\sqrt{2}}{2}$. 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, $\sqrt{\frac{n_u(u_i,x_i,O_{2k+1})+n_v(u_i,x_i,O_{2k+1})-2}{n_u(u_i,x_i,O_{2k+1})n_v(u_i,x_i,O_{2k+1})}} = \sqrt{\frac{6k+2}{(6k-3i+5)(3i-1)}}$. 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 $x_i$ than $u_i$, 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, $\sum_{uv \in A} \sqrt{\frac{n_u(u,v,O_{2k+1})+n_v(u,v,O_{2k+1})-2}{n_u(u,v,O_{2k+1})n_v(u,v,O_{2k+1})}} = 2\sqrt{\frac{6k+2}{3k+2}} + \sqrt{2}$, 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:

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

Therefore, we have the result.

(ii) It follows from Theorem 3.2

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 $n = 2k$, we have:

$$ABC_{GG}(O_n^h) = 4 \left( \sum_{i=1}^{k} \sqrt{\frac{10k-1}{(10k-5i+3)(5i-2)}} \right) + 8k \sqrt{\frac{10k-1}{30k-6}}.$$
Figure 13: Para-chain square cactus $O_{2k+1}$.

Figure 14: Ortho-chain graph $O^h_n$.

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

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

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

Proof.

(i) It is similar to the proof of Theorem 3.5.

(ii) It follows from Theorem 3.2. □

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:

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

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Figure 15: Para-chain hexagonal graph $L_n$.

(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. □

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 $n = 2k + 1$, 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.
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

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

and we have the result. \hfill \square

**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. \hfill \square

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

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 \( x_0 \) than \( x_1 \), and there are \( 2^n - 1 \) vertices
closer to $x_1$ than $x_o$. So, \[ \sqrt{\frac{n_{x_0}(x_0 x_1, T_n) + n_{x_1}(x_0 x_1, T_n) - 2}{n_{x_0}(x_0 x_1, T_n)n_{x_1}(x_0 x_1, T_n)}} = \sqrt{\frac{2^{n+2} + 2^{n-4}}{(2^{n+2} - 1)(2^{n-1})}}. \] The edge $ax_0$ has the same attitude as the blue edge $x_0 x_1$. 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, \[ \sqrt{\frac{n_{a}(ax_1, T_n) + n_{x_1}(ax_1, T_n) - 2}{n_{a}(ax_1, T_n)n_{x_1}(ax_1, T_n)}} = \sqrt{\frac{2^{n+1} - 1}{2^n - 1}}, \] and in total, we have 3 edges like this one.

Now consider the edge $x_1 x_2$. 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, \[ \sqrt{\frac{n_{x_0}(x_0 x_1, T_n) + n_{x_1}(x_0 x_1, T_n) - 2}{n_{x_0}(x_0 x_1, T_n)n_{x_1}(x_0 x_1, T_n)}} = \sqrt{\frac{2^{n+2} + 2^n + 2^{n-1} - 4}{(2^{n+2} + 2^n + 2^{n-1} - 1)(2^{n-1} - 1)}}. \] The edge $bx_1$ has the same attitude as the red edge $x_1 x_2$. 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, \[ \sqrt{\frac{n_{b}(bx_1, T_n) + n_{x_1}(bx_1, T_n) - 2}{n_{b}(bx_1, T_n)n_{x_1}(bx_1, T_n)}} = \sqrt{\frac{2^{n+1} - 4}{2^n - 1}}, \] and in total, we have 6 edges like this one.

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

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

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, \[ \sqrt{\frac{n_l(lx_1, T_n) + n_{x_1}(lx_1, T_n) - 2}{n_l(lx_1, T_n)n_{x_1}(lx_1, T_n)}} = \sqrt{\frac{2^{n+i+2} - 4}{2^{n-i+1} - 1}}, \] 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

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

and therefore we have the result. \(\square\)

![Image of Graph T_n](image)

Figure 20: Graph \(T_n\).

### 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).

**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

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

and we have the result. \qed
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