Abstract. Among topological descriptors connectivity indices are very important and they have a prominent role in chemistry. Two useful of them are the geometric-arithmetic (GA) and atom-bond connectivity (ABC) indices and are defined as $GA(G) = \sum_{uv \in E(G)} \frac{2\sqrt{d_u d_v}}{d_u + d_v}$ and $ABC(G) = \sum_{e=uv \in E(G)} \sqrt{\frac{d_u + d_v - 2}{d_u d_v}}$, in which $d_u$ and $d_v$ are the degrees of the vertices $u$ and $v$, respectively. In this paper we compute these connectivity topological indices for a special chemical molecular graph “Cas(C)-CaR(C)[m,n,p] Nanotubes Junction” are given. The Cas(C)-CaR(C)[m,n,p] Nanotubes Junction is a new nano-structure that was defined by M.V. Diudea, on based the new graph operations (Leapfrog Le and Capra Ca) on the cycle graph $C_n$.

Keywords. Molecular graph; Nanotubes; geometric-arithmetic (GA) index, atom-bond connectivity (ABC) index

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1. Introduction

A graph is a collection of points and lines connecting a subset of them. The points and lines of a graph also called vertices and edges of the graph, respectively. In chemical graphs, the vertices and edges of a graph also correspond to the atoms and bonds of the molecular graph, respectively. If \( e \) is an edge/bond of \( G \), connecting the vertices/atoms \( u \) and \( v \), then we write \( e = uv \) and say “\( u \) and \( v \) are adjacent” [16–27]. The graph \( G \) is said to be connected, if for every vertices \( u \) and \( v \) in \( V(G) \) there exists a path connecting \( u \) and \( v \).

Chemical graph theory is an important branch of graph theory, such that there exits many topological indices in it. The topological indices of the graph \( G \) are a number relation to the structure of the graph \( G \) and are invariant on the automorphism of the graph. The simplest topological indices are the number of vertices, the number of edges and degree of a vertex \( v \) of the graph \( G \) and we denoted by \( n, m \) and \( d_v \), respectively. The degree of a vertex \( v \) is the number of vertices joining to \( v \) and the distance \( d(u, v) \) in a graph is the number of edges in a shortest path connecting them.

One of the oldest topological indices is the Wiener index \( W(G) \), introduced by the chemist Harold Wiener [27] in 1947. It is defined as the sum of topological distances \( d(u, v) \) between any two atoms in the molecular graph

\[
W(G) = \frac{1}{2} \sum_{u \in V(G)} \sum_{v \in V(G)} d(u, v).
\]

Let \( G \) be a (molecular) graph with vertex and edge sets being denoted by \( V(G) \) and \( E(G) \), respectively. B. Furtula et al. introduced Atom-Bond Connectivity index (ABC) and Geometric-Arithmetic index (GA) [16,25]. These indices are based on degrees of vertices and defined as follow, respectively.

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

\[
GA(G) = \sum_{e = uv \in E(G)} \frac{2\sqrt{d_u d_v}}{d_u + d_v},
\]

where \( d_u \) and \( d_v \) are the degrees of the vertices \( u \) and \( v \), respectively. In all parts of this paper, our notation is standard and mainly taken from standard books of chemical graph theory [6–27].

2. Main Results

In this paper, we investigate the above presented topological Connectivity indices in a family of special chemical molecular graphs “Cas(C)-CaR(C)[m,n,p] Nanotubes Junction” (see Figure 1).

The Cas(C)-CaR(C)[m,n,p] Nanotubes Junction is a new nano-structure that was defined by M.V. Diudea [1], on based the new graph operations on the cycle graph \( C_n \), namely: Leapfrog Le and Capra Ca. Some examples of graph operations (Leapfrog Le and Capra Ca) are shown in Figure 2 and Figure 3 and readers can see the references [2–15].
Figure 1. [1–5] A-dimensional lattice of $\text{Cas}(C)\text{-CaR}(C)[m, n, p]$ Nanotubes Junction $\forall m, n, p \in \mathbb{N}$.

Figure 2. [1–5] An example of “Leapfrog Le($C_6$)” graph operation.

Now, consider $\text{Cas}(C)\text{-CaR}(C)[m, n, p]$ Nanotubes Junction $\forall m, n, p \in \mathbb{N}$, such that the 3-Dimensional lattice of $\text{Cas}(C)\text{-CaR}(C)[m, n, p]$ Nanotubes Junction are shown in Figure 1. In this paper we name the first member $\text{Cas}(C)[1, 1, 1]$ or $\text{Cas}(C)$ as the based unit (see Figure 4), since all member of $\text{Cas}(C)[m, n, p]$ Nanotubes are combine this unit.

By Figure 4, we can see that $6 \times 4 = 24$ vertices/atoms of $\text{Cas}(C)$ unit have degree 2 (red colored vertices in Figure 3), and there are $2 \times 4 = 8$ vertices/atoms with degree 3 in any split of $\text{Cas}(C)$ (yellow colored vertices in Figure 3) and $\text{Cas}(C)$ unit has 6 splits. Finally, there are 8 common vertices between 3 joist splits of $\text{Cas}(C)$ (obviously with degree 3 and colored by white).
These imply that $\text{Cas}(C)$ unit has $24 + 6 \times 8 + 8 = 80$ ($|V(\text{Cas}(C))|$) vertices/atoms and the number of edges/bonds of $\text{Cas}(C)$ unit is equal to

$$|E(\text{Cas}(C))| = \frac{2 \times |V_2| + 3 \times |V_3|}{2} = \frac{1}{2} [2 \times 24 + 3 \times 56] = 216.$$

Thus following M.V. Diudea [5] we denote the number of $\text{Cas}(C)$ units in the first rows and column in this Nanotube by integer number $m$, $n$ and $p$. Therefore, in general case of this nano-structure $\text{Cas}(C)-\text{CaR}(C)[m,n,p]$, there are $m \times n \times p \text{Cas}(C)$ units and there exist $|V(\text{Cas}(C)-\text{CaR}(C)[m,n,p])| = 80 \times m \times n \times p = 80mn\ p \text{ number of vertices/atoms (} \forall \ m,n,p \in \mathbb{N}).$

Also, from the structure of $\text{Cas}(C)-\text{CaR}(C)[m,n,p]$ Nanotubes Junction $\forall \ m,n,p \in \mathbb{N}$, in Figure 4, one can see that the number of edges/bonds of $\text{Cas}(C)-\text{CaR}(C)[m,n,p]$ is equal to

$$|E(\text{Cas}(C)-\text{CaR}(C)[m,n,p])| = 216 \times m \times n \times p + 4(m - 1)(n - 1)(p - 1)$$

$$= 220mn\ p - 4mn - 4mp - 4np + 4m + 4n + 4p - 4.$$

Before presenting the main results, let us introduce some definitions.
Definition 1 ([16–18]). Let $G$ and $d_v$ ($1 \leq d_v \leq n - 1$) be a simple connected molecular graph and the vertex degrees of vertices/atom $v$ in $G$. We divide the vertex set $V(G)$ and edge set $E(G)$ of $G$ into several partitions based on $d_v$ ($\forall v \in V(G)$) for $\delta \leq k \leq \Delta$, $2\delta \leq i \leq 2\Delta$, and $\delta^2 \leq j \leq \Delta^2$ as follows

\[
\begin{align*}
V_k &= \{v \in V(G) | d_v = k\}, \\
E_i &= \{e = uv \in E(G) | d_u + d_v = i\}, \\
E_j^* &= \{uv \in E(G) | d_u \times d_v = j\},
\end{align*}
\]

where $\delta$ and $\Delta$ are the minimum and maximum, respectively, of $d_v$ for all $v \in V(G)$.

In any nanostructure, the degree of an arbitrary vertex/atom of a molecular graph is equal to 1, 2 or 3. Also, the hydrogen atoms in molecular graphs (i.e., vertices of degree 1) are often omitted. Therefore in the case $G = Cas(C)$ unit, we have only

\[
\begin{align*}
V_3 &= \{v \in V(Cas(C)) | d_v = 3\}, \\
V_2 &= \{v \in V(Cas(C)) | d_v = 2\}.
\end{align*}
\]

Because $\forall v \in V(Cas(C))d_v = 2$ or 3, and alternatively the edge partitions of $Cas(C)$ are as

\[
\begin{align*}
E_5 &= E_5^* = \{uv \in E(Cas(C)) | d_u = 2 \text{ and } d_v = 3\}, \\
E_6 &= E_6^* = \{uv \in E(Cas(C)) | d_u = d_v = 3\}.
\end{align*}
\]

By according to the Figure 4, it’s easy to see that the cardinal of these vertex and edge partitions are equal to:

| Vertex/Edge partition | $V_3$ | $V_2$ | $E_5 = E_6^*$ | $E_6 = E_9^*$ |
|-----------------------|-------|-------|----------------|----------------|
| Cardinality           | 56    | 24    | $2 \times |V_2| = 48$ | 168 |

By these preliminaries, we have main results of this paper in following theorems.

Theorem 1. Let $G$ be the general case of the nano-structure “Cas(C)–CaR(C)[$m,n,p$] Nanotubes Junction” (see Figure 1). Then,

- the atom-bond connectivity index $ABC$ of $G$ is equal to
  \[ABC(Cas(C)–CaR(C)[m,n,p]) = \frac{440}{3} mnp + \left(8\sqrt{2} - \frac{40}{3}\right)(mp + np + mn) + \frac{8}{3}(m + n + p - 1),\]

- the geometric-arithmetic $GA$ of $G$ is equal to
  \[GA(Cas(C)–CaR(C)[m,n,p]) = 220 mnp + \left(32 \sqrt{6} - 20\right)(mp + np + mn) + 4(m + n + p - 1).\]

Proof. Consider $G = Cas(C)–CaR(C)[m,n,p]$ nano-structure. This nano-structure consists of heptagon and octagon nets (see Figure 1). By above mention results, one can see that the vertex and edge sets of $G$ are equal to ($\forall m,n,p \in \mathbb{N}$):

\[|V(Cas(C)–CaR(C)[m,n,p])| = 10(2m)(2n)(2P),\]
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\[ |E(Cas(C) - CaR(C)[m, n, p])| = 220 mnp - 4mn - 4mp - 4np + 4m + 4n + 4p - 4. \]

In the general case \( G = Cas(C) - CaR(C)[m, n, p] \) Nanotubes Junction, we can see that \( \forall v \in V(Cas(C) - CaR(C)[m, n, p]) \) \( d_v = 2 \) or \( 3 \), and we have the vertex and edge partitions with their cardinalities as follows (\( \forall m, n, p \in \mathbb{N} \)).

\[
V_3 = \{v \in V(G) | d_v = 3\}, \\
V_2 = \{v \in V(G) | d_v = 2\}.
\]

| Vertex partition | \( V_2 \) | \( V_3 \) |
|------------------|-----------|-----------|
| Cardinality      | \( 4(2mp + 2np + 2mn) \) | \( 8(10mnp - mnp - np - mn) \) |

\[ E_5^* = E_6^* = \{uv \in E(G) | d_u = 2 \text{ and } d_v = 3\}, \]
\[ E_6^* = E_9^* = \{uv \in E(G) | d_u = d_v = 3\}. \]

| Edge partition | \( E_5^* = E_6^* \) | \( E_6^* = E_9^* \) |
|----------------|---------------------|---------------------|
| Cardinality    | \( 16(mp + np + mn) \) | \( 4(55mnp - 5mn - 5mp - 5np + m + n + p - 1) \) |

Then, we have following computations for the geometric-arithmetic (GA) and atom-bond connectivity (ABC) indices of \( Cas(C) - CaR(C)[m, n, p] \) Nanotubes Junction (\( \forall m, n, p \in \mathbb{N} \)).

\[
ABC(G) = \sum_{uv \in E(G)} \sqrt{\frac{d_u + d_v - 2}{d_ud_v}} \\
= \sum_{u_1v_1 \in E_9^*} \sqrt{\frac{d_{u_1} + d_{v_1} - 2}{d_{u_1}d_{v_1}}} + \sum_{u_2v_2 \in E_6^*} \sqrt{\frac{d_{u_2} + d_{v_2} - 2}{d_{u_2}d_{v_2}}} \\
= \frac{2}{3} |E_9^*| + \frac{\sqrt{2}}{2} |E_6^*| \\
= \frac{2}{3} (220 mnp - 20mn - 20mp - 20np + 4m + 4n + 4p - 4) + \frac{\sqrt{2}}{2} (8(2mp + 2np + 2mn)) \\
= \frac{8}{3} (55mnp - 5mn - 5mp - 5np + m + n + p - 1) + 8\sqrt{2}(mp + np + mn) \\
= \frac{440}{3} mn + \left(8\sqrt{2} - \frac{40}{3}\right) (mp + np + mn) + \frac{8}{3} (m + n + p - 1)
\]

and also,

\[
GA(G) = \sum_{uv \in E(G)} \frac{2\sqrt{d_ud_v}}{d_u + d_v} \\
= \sum_{u_1v_1 \in E_9^*} \frac{2\sqrt{d_{u_1}d_{v_1}}}{d_{u_1} + d_{v_1}} + \sum_{u_2v_2 \in E_6^*} \frac{2\sqrt{d_{u_2}d_{v_2}}}{d_{u_2} + d_{v_2}} \\
= \frac{2\sqrt{6}}{6} |E_9^*| + \frac{2\sqrt{6}}{5} |E_6^*| \\
= 4(55mnp - 5mn - 5mp - 5np + m + n + p - 1) + \frac{2\sqrt{6}}{5} (16(mp + np + mn))
\]
\[ = 220mnp + \left( \frac{32\sqrt{6}}{5} - 20 \right) (m p + n p + m n) + 4(m + n + p - 1). \]

and this completed the proof.

### 3. Conclusion

In this study we have calculated the geometric-arithmetic (GA) and atom-bond connectivity (ABC) indices of a special chemical molecular graph “Cas(C)-CaR(C)[m,n,p] Nanotubes Junction” are given. The Cas(C)-CaR(C)[m,n,p] Nanotubes Junction is a new nano-structure that was defined by M.V. Diudea, on based the new graph operations (Leapfrog Le and Capra Ca) on the cycle graph \( C_n \).

### Competing Interests

The authors declare that they have no competing interests.

### Authors’ Contributions

All the authors contributed significantly in writing this article. The authors read and approved the final manuscript.

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