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SOME NUMERICAL INVARIANTS ASSOCIATED WITH V-PHENYLENIC NANOTUBE AND NANOTORI

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Abstract. A carbon nanotube (CNT) is a miniature cylindrical carbon structure that has hexagonal graphite molecules attached at the edges. In this paper, we compute the numerical invariant (Topological indices) of linear [n]-phenylenic, lattice of $C_4C_6C_8[m,n]$, $TUC_4C_6C_8[m,n]$ nanotube, $C_4C_6C_8[m,n]$ nanotori.

Index Terms: Molecular graph; topological index; nanotube; nanotori.

1. Introduction

Mathematical chemistry is a branch of theoretical chemistry for discussion and prediction of the molecular structure using mathematical methods without necessarily referring to quantum mechanics. Chemical graph theory is a branch of mathematical chemistry which applies graph theory to mathematical modelling of chemical phenomena [1, 2]. This theory had an important effect on the development of the chemical sciences. In mathematics chemistry, a molecular graph is a simple graph such that its vertices correspond to the atoms and the edges to the bonds. And also a connected graph is a graph such that there is a path between all pairs of vertices. Note that hydrogen atoms are often omitted [2]. Let $G = (V, E)$ be a graph with n vertices and m edges. The degree of a vertex $u \in V(G)$ is denoted by $d_G(u)$ and is the number of vertices that are adjacent to u. The edge connecting the vertices u and v is denoted by uv [3].

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2. Computing the Topological Indices of Certain Nanotubes

In [4, 5, 6], Shigehalli and Kanabur have put forward new degree based topological indices viz. arithmetic-geometric index, SK index, SK_1 index and SK_2 index. Which are defined as follows: Let $G = (V, E)$ be a molecular graph,$d_G(u)$ and , $d_G(v)$ is the degree of the vertex u and v, then

$$AG_1 = \sum_{uv \in E(G)} \frac{1}{2\sqrt{d_u + d_v}}, \quad (1)$$

$$SK = \sum_{uv \in E(G)} \frac{d_u + d_v}{2}, \quad (2)$$

$$SK_1 = \sum_{uv \in E(G)} \frac{d_u d_v}{2}, \quad (3)$$

$$SK_2 = \sum_{uv \in E(G)} \left(\frac{d_u + d_v}{2}\right)^2. \quad (4)$$

where $d_G(u)$ and $d_G(v)$ are the degrees of the vertices u and v in G. In this paper we give explicit formulae for these topological indices of [n]-phenylenic, lattice of $C_4C_6C_8[m, n]$, $TUC_4C_6C_8[m, n]$ nanotube, $C_4C_6C_8[m, n]$ nanotori [7, 8].

3. Main Results

The aim of this section, at first, is to compute some topological indices of the molecular graph of linear[n]-phenylenic as depicted in Fig.1

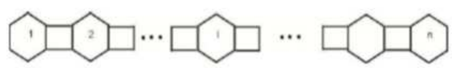

Figure 1. The molecular graph of a linear [n]-phenylenic.

It is easy to see that $T = T[n]$ has 6n vertices and $8n - 2$ edges, We partition the edges of T into three subsets $E_1(T)$, $E_2(T)$ and $E_3(T)$, Table1 shows the number of three types of edges.

TABLE 1. The number of three types of edges of the graph T.

(d_u, d_v)	Number of edges
(2,2)	6
(2,3)	$4n - 4$
(3,3)	$4n - 4$

From this table, we given an explicit computing formula for some indices of a linear [n]-phenylenic, as shown in above graph.

Theorem 3.1. *Consider the graph T of a linear[n]-phenylenic. Then the AG_1, SK, SK_1 and SK_2 indices of T are equal to*

(1) $AG_1(G) = 8.08n - 2.08$,
(2) $SK(G) = 22n - 10$,
(3) $SK_1(G) = 30n - 18$,
(4) $SK_2(G) = 61n - 37$.

Proof. (1)

$$\begin{aligned}
AG_1(G) &= \sum_{uv \in E(G)} \frac{d_u + d_v}{2\sqrt{d_u.d_v}} \\
&= \sum_{uv \in E_1(G)} \frac{d_u + d_v}{2\sqrt{d_u.d_v}} + \sum_{uv \in E_2(G)} \frac{d_u + d_v}{2\sqrt{d_u.d_v}} \\
&\quad + \sum_{uv \in E_3(G)} \frac{d_u + d_v}{2\sqrt{d_u.d_v}} \\
&= |E_1(G)|\frac{2+2}{2\sqrt{2.2}} + |E_2(G)|\frac{2+3}{2\sqrt{2.3}} \\
&\quad + |E_3(G)|\frac{3+3}{2\sqrt{3.3}} \\
&= 6(1) + (4n-4)\left(\frac{5}{2\sqrt{6}}\right) + (4n-4)(1) \\
&= 8.08n - 2.08.
\end{aligned}$$

(2)

$$\begin{aligned}
SK(G) &= \sum_{uv \in E(G)} \frac{d_u + d_v}{2} \\
&= \sum_{uv \in E_1(G)} \frac{d_u + d_v}{2} + \sum_{uv \in E_2(G)} \frac{d_u + d_v}{2} \\
&\quad + \sum_{uv \in E_3(G)} \frac{d_u + d_v}{2} \\
&= |E_1(G)|\frac{2+2}{2} + |E_2(G)|\frac{2+3}{2} \\
&\quad + |E_3(G)|\frac{3+3}{2} \\
&= 12 + 10n - 10 + 12n - 12 \\
&= 22n - 10.
\end{aligned}$$

(3)

$$SK_1(G) = \sum_{uv \in E(G)} \frac{d_u d_v}{2}$$

$$\begin{aligned} &= \sum_{uv\in E_1(G)} \frac{d_u d_v}{2} + \sum_{uv\in E_2(G)} \frac{d_u d_v}{2} \\ &\quad + \sum_{uv\in E_3(G)} \frac{d_u d_v}{2} \\ &= |E_1(G)|\frac{2.2}{2} + |E_2(G)|\frac{2.3}{2} \\ &\quad +|E_3(G)|\frac{3.3}{2} \\ &= = 12 + 12n - 12 + 18n - 18 \\ &= 30n - 18. \end{aligned}$$

(4)

$$\begin{aligned} SK_2(G) &= \sum_{uv\in E(G)} \left(\frac{d_u + d_v}{2}\right)^2 \\ &= \sum_{uv\in E_1(G)} \left(\frac{d_u + d_v}{2}\right)^2 + \sum_{uv\in E_2(G)} \left(\frac{d_u + d_v}{2}\right)^2 \\ &\quad + \sum_{uv\in E_3(G)} \left(\frac{d_u + d_v}{2}\right)^2 \\ &= |E_1(G)|\left(\frac{2+2}{2}\right)^2 + |E_2(G)|\left(\frac{2+3}{2}\right)^2 \\ &\quad +|E_3(G)|\left(\frac{3+3}{2}\right)^2 \\ &= 24 + 25n - 25 + 36n - 36 \\ &= 61n - 37. \end{aligned}$$

□

In continue of this section, we see the following figures

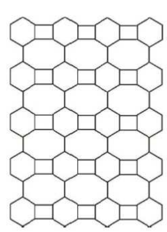

Figure 2. The 2-D graph lattice of $C_4C_6C_8[4, 5]$ nanotube.

We now consider the molecular graph $G = C_4C_6C_8[m, n]$, Fig.2. It is easy to see that $|V(G)| = 6mn$ and $|E(G)| = 9mn - 2n - m$, We partition the edges of

G into three subsets $E_1(G)$, $E_2(G)$ and $E_3(G)$. The number of three types of edges is shown in Table 2.

TABLE 2. The number of three types of edges of the graph T.

(d_u, d_v)	Number of edges
(2,2)	$2n+4$
(2,3)	$4m+4n-8$
(3,3)	$9mn-8n-5m+4$

From this table, we have given an explicit computing of some indices of G (Fig. 2).

Theorem 3.2. *Consider the graph T of a linear[n]-phenylenic. Then the AG_1, SK, SK_1 and SK_2 indices of T are equal to*

(1) $AG_1(G) = (9n-5.92)m - 9.92n - 3.84$,
(2) $SK(G) = (27n-5)m - 10n$,
(3) $SK_1(G) = (40.5n-10)m - 20n + 2$,
(4) $SK_2(G) = (81n-20)m - 39n - 48$.

Proof. (1)

$$\begin{aligned}
AG_1(G) &= \sum_{uv\in E(G)} \frac{d_u+d_v}{2\sqrt{d_u.d_v}} \\
&= \sum_{uv\in E_1(G)} \frac{d_u+d_v}{2\sqrt{d_u.d_v}} + \sum_{uv\in E_2(G)} \frac{d_u+d_v}{2\sqrt{d_u.d_v}} \\
&\quad + \sum_{uv\in E_3(G)} \frac{d_u+d_v}{2\sqrt{d_u.d_v}} \\
&= |E_1(G)|\frac{2+2}{2\sqrt{2.2}} + |E_2(G)|\frac{2+3}{2\sqrt{2.3}} \\
&\quad +|E_3(G)|\frac{3+3}{2\sqrt{3.3}} \\
&= 9mn - 5.92m - 9.92n - 3.04 \\
&= = (9n-5.92)m - 9.92n - 3.84.
\end{aligned}$$

(2)

$$\begin{aligned}
SK(G) &= \sum_{uv\in E(G)} \frac{d_u+d_v}{2} \\
&= \sum_{uv\in E_1(G)} \frac{d_u+d_v}{2} + \sum_{uv\in E_2(G)} \frac{d_u+d_v}{2} \\
&\quad + \sum_{uv\in E_3(G)} \frac{d_u+d_v}{2}
\end{aligned}$$

$$
\begin{aligned}
&= |E_1(G)|\frac{2+2}{2} + |E_2(G)|\frac{2+3}{2} \\
&\quad +|E_3(G)|\frac{3+3}{2} \\
&= = 4n + 8 + 10m + 10n - 20 + 27mn - 24n - 15m + 12 \\
&= 27mn - 10n - 5m.
\end{aligned}
$$

(3)

$$
\begin{aligned}
SK_1(G) &= \sum_{uv\in E(G)} \frac{d_u d_v}{2} \\
&= \sum_{uv\in E_1(G)} \frac{d_u d_v}{2} + \sum_{uv\in E_2(G)} \frac{d_u d_v}{2} \\
&\quad + \sum_{uv\in E_3(G)} \frac{d_u d_v}{2} \\
&= |E_1(G)|\frac{2.2}{2} + |E_2(G)|\frac{2.3}{2} \\
&\quad +|E_3(G)|\frac{3.3}{2} \\
&= = 4n + 8 + 12m + 12n - 24 + 40.5mn - 36n - 22.5m + 8 \\
&= (40.5n - 10)m - 20n + 2.
\end{aligned}
$$

(4)

$$
\begin{aligned}
SK_2(G) &= \sum_{uv\in E(G)} \left(\frac{d_u + d_v}{2}\right)^2 \\
&= \sum_{uv\in E_1(G)} \left(\frac{d_u + d_v}{2}\right)^2 + \sum_{uv\in E_2(G)} \left(\frac{d_u + d_v}{2}\right)^2 \\
&\quad + \sum_{uv\in E_3(G)} \left(\frac{d_u + d_v}{2}\right)^2 \\
&= |E_1(G)| \left(\frac{2+2}{2}\right)^2 + |E_2(G)| \left(\frac{2+3}{2}\right)^2 \\
&\quad +|E_3(G)| \left(\frac{3+3}{2}\right)^2 \\
&= 8n + 16 + 25m + 25n - 100 + 81mn - 72n - 45m + 36 \\
&= (81n - 20)m - 39n - 48.
\end{aligned}
$$

□

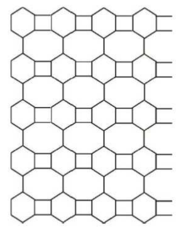

Figure 3. The 2-D graph lattice of $TUC_4C_6C_8[4,5]$ nanotube.

We now consider the molecular graph $K = TUC_4C_6C_8[m,n]$, Fig. 3. It is easy to see that $|V(K)| = 6mn$ and $|E(K)| = 9mn - n$. We partition the edges of nanotube K into two subsets $E_1(G)$, $E_2(G)$ and compute the total number of edges for the 2-dimensional of graph K (Table 3).

TABLE 3. The number of three types of edges of the graph T.

(d_u, d_v)	Number of edges
(2,3)	$4n$
(3,3)	$9mn - 5m$

From this table, we given an explicit computing formula for some indices of a linear [n]-phenylenic, as shown in above graph.

Theorem 3.3. *Consider the graph T of a linear[n]-phenylenic. Then the AG_1, SK, SK_1 and SK_2 indices of T are equal to*

(1) $AG_1(G) = (9n - 0.92)m$,
(2) $SK(G) = (27n - 5)m.$,
(3) $SK_1(G) = (40.5n - 10.5)m.$,
(4) $SK_2(G) = (81n - 20)m..$

Proof. (1)

$$\begin{aligned} AG_1(G) &= \sum_{uv\in E(G)} \frac{d_u + d_v}{2\sqrt{d_u.d_v}} \\ &= \sum_{uv\in E_1(G)} \frac{d_u + d_v}{2\sqrt{d_u.d_v}} + \sum_{uv\in E_2(G)} \frac{d_u + d_v}{2\sqrt{d_u.d_v}} \\ &= |E_1(G)|\frac{2+3}{2\sqrt{2.2}} + |E_2(G)|\frac{3+3}{2\sqrt{2.3}} \\ &= 9mn - 5m + 4.08m \\ &= (9n - 0.92)m. \end{aligned}$$

(2)

$$SK(G) = \sum_{uv\in E(G)} \frac{d_u + d_v}{2}$$

$$
\begin{aligned}
&= \sum_{uv\in E_1(G)} \frac{d_u+d_v}{2} + \sum_{uv\in E_2(G)} \frac{d_u+d_v}{2} \\
&= |E_1(G)|\frac{2+3}{2} + |E_2(G)|\frac{3+3}{2} \\
&= 10m + 27mn - 15m \\
&= (27n-5)m.
\end{aligned}
$$

(3)

$$
\begin{aligned}
SK_1(G) &= \sum_{uv\in E(G)} \frac{d_u d_v}{2} \\
&= \sum_{uv\in E_1(G)} \frac{d_u d_v}{2} + \sum_{uv\in E_2(G)} \frac{d_u d_v}{2} \\
&= |E_1(G)|\frac{2.3}{2} + |E_2(G)|\frac{3.3}{2} \\
&= = 12mn + (9mn - 5m)(4.5) \\
&= (40.5n - 10.5)m.
\end{aligned}
$$

(4)

$$
\begin{aligned}
SK_2(G) &= \sum_{uv\in E(G)} \left(\frac{d_u+d_v}{2}\right)^2 \\
&= \sum_{uv\in E_1(G)} \left(\frac{d_u+d_v}{2}\right)^2 + \sum_{uv\in E_2(G)} \left(\frac{d_u+d_v}{2}\right)^2 \\
&= |E_1(G)|\left(\frac{2+3}{2}\right)^2 + |E_2(G)|\left(\frac{3+3}{2}\right)^2 \\
&= 25m + 81mn - 45m \\
&= (81n-20)m.
\end{aligned}
$$

□

4. conclusion

In this paper, we have computed the value of AG_1 index, SK index, SK_1 index and SK_2 index for Linear [n]-phenylenic, lattice of $C_4C_6C_8[m,n]$, $TUC_4C_6C_8[m,n]$ nanotube, $C_4C_6C_8[m,n]$ nanotori without using computer.

Competing Interests

The authors declare that they have no competing interests.

References

1. Diudea, M. V., Gutman, I., & Jantschi, L. (2001). *Molecular topology.* Huntington, NY: Nova Science Publishers.
2. Trinajstić, N. (1992). *Chemical Graph Theory*, CRC Press. Boca Raton.
3. Harary, F. (1969). *Graph theory. Addison-Wesely, Reading mass.*
4. Shigehalli, V. S., & Kanabur, R. (2016). New Version of Degree-Based Topological Indices of Certain nanotube. *J. Math. Nanosci,* 6(1), 29-42.
5. Shigehalli, V. S., & Kanabur, R. (2016). Computation of new degree-based topological indices of graphene. *Journal of Mathematics*, 2016.
6. Shigehalli, V., & Kanabur, R. (2016). Computing degree-based topological indices of Polyhex nanotubes. *Journal of Mathematical Nanoscience*, 6(1-2), 47-55.
7. Nikmehr, M. J., Veylaki, M., & Soleimani, N. (2015). Some topological indices of V-Phenylenic nanotube and nanotori. *Optoelectron. Adv. Mater.-Rapid Comm*, 9(9), 1147-1149.
8. Hosamani, S. M., & Gutman, I. (2014). Zagreb indices of transformation graphs and total transformation graphs. *Applied Mathematics and Computation*, 247, 1156-1160.

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