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On computation of some distance-based topological indices of circulant networks

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Abstract

The distance, $d(u, v)$, between two vertices u and v of a connected graph G is the length of a $u - v$ geodesic in G. A large number of graph-distance-based topological indices in various families of graphs and networks have been computed. In this paper, we consider circulant networks and compute three distance-based topological indices, namely the Wiener index, hyper-Wiener index and Schultz molecular topological index on these networks.

Keywords: Wiener index, hyper-Wiener index and Schultz index, circulant network.

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1. Preliminaries

A combination of chemistry, mathematics and information defines a new subject called cheminformatics. To predict the biological activities and properties of chemical compounds, cheminformatics studies Quantitative structure-activity and Quantitative structure-property relationships (QSAR/QSPR). In QSAR/QSPR study, physico-chemical properties and topological indices such as Wiener index, hyper-Wiener index, Harary index, Randić index, Zagreb index and Schultz index are used to predict bioactivity of chemical compounds.

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Let $\mathcal{G}$ be a family of graphs. A topological index is a function $Top : \mathcal{G} \to \mathbb{R}$ such that $G \cong H$ implies $Top(G) = Top(H)$ for two graphs $G, H \in \mathcal{G}$ [8]. A topological index is, in fact, a numeric quantity associated with chemical constitution purporting for correlation of chemical structure with many physico-chemical properties. Actually, they are designed on the ground of transformation of a molecular graph into a number which characterizes the topology of that graph. Due to the chemical significance of topological indices, remarkable research has been done on topological indices of various families of graphs.

In this paper, we consider simple connected graphs G with vertex set $V(G)$ and edge set $E(G)$. The number $d(v)$ denotes the *degree* of a vertex v in G, which is the number of edges adjacent with v in G. The number $d(u, v)$ denotes the *distance* between two vertices u and v of G, which is defined as the length of a shortest path between u and v in G. A network is simply a connected graph having no multiple edges. Here, we consider the family of circulant networks, which is defined as follows: Let n, m and $a_1, a_2, \ldots, a_m$ be positive integers, $1 \leq a_i \leq \lfloor \frac{n}{2} \rfloor$ and $a_i \neq a_j$ for all $1 \leq i < j \leq m$. An undirected graph with the set of vertices $\{v_{i+1} \ ; \ i \in Z_n\}$ (Z_n : the additive group of integers modulo n) and the set of edges $\{v_j v_{j+a_l} : \ 1 \leq j \leq n, 1 \leq l \leq m\}$ is called a *circulant graph*, and is denoted by $C_n(a_1, a_2, \ldots, a_m)$. The numbers $a_1, a_2, \ldots, a_m$ are called the generators and we say that the edge $v_j v_{j+a_l}$ is of type a_l. The indices after n will be taken modulo n. It is easy to see that a circulant network $C_n(a_1, a_2, \ldots, a_m)$ is a regular graph of degree r, where

$$r = \begin{cases} 2m - 1 & \text{if } \frac{n}{2} \in \{a_1, a_2, \ldots, a_m\}, \\ 2m & \text{otherwise.} \end{cases}$$

The class of circulant networks is an important class of graphs, which is useful in the design of local area networks [1]. Circulant networks have played a vital role for decades in the design of computer and telecommunication networks due to their optimal fault-tolerance and routing capabilities [2]. They also constitute the basis for designing certain data alignment networks for complex memory systems [14]. We consider two families of circulant graphs, $C_n(1, a)$ for $a = 2, 3$ in this paper, and compute the Wiener, hyper-Wiener and Schultz indices on these families, which are defined as follows:

In 1947, to study the boiling points of paraffins, Wiener introduced the first non-trivial distance-based topological index. He named this index the *path number*, and later on it was called the *Wiener index* [13]. The research interest in Wiener index and related indices is still considerable (see the bibliography and therein [9, 11]). This index was given in terms of edge weights which, originally, was defined on trees. Traditionally, its generalization on general graphs G is defined as:

$$W(G) = \sum_{u,v \in V(G)} d(u, v).$$

During the last two decades, a large number of generalizations and extensions of the Wiener index has been introduced and studied by various mathematical chemists. An extensive bibliography on this matter can by viewed in [4, 7]. One of these extensions, the *hyper-Wiener index* was proposed by Randić for trees [10], and extended to all connected graphs by Klein *et al.* [6]. This index remarkably used as a structure descriptor for predicting physicochemical properties of chemical compounds, which are significant for pharmacology, agriculture and environment protection [3, 6, 10]. This index is defined as:

$$WW(G) = \frac{1}{2} \sum_{u,v \in V(G)} d(u, v)(1 + d(u, v)).$$

Another generalization of the Wiener index is the *Schultz molecular topological index*, which was introduced in 1989 [12], and is defined as:

$$MTI(G) = \sum_{u\in V(G)} \sum_{v\in V(G)} d(u)(A_{uv} + d(u,v)),$$

where A_{uv} is the (u,v)-th entry of the adjacency matrix A of G.

2. Circulant networks $C_n(1,2)$

In this section, we consider circulant networks $C_n(1,2)$, for all $n \geq 5$, in the context of the Wiener, hyper-Wiener and Schultz indices. Firstly, we define some notations which will be useful in the sequel. Let

$$D(v|G) = \sum_{u\in V(G)} d(u,v) \quad \text{and} \quad DD(v|G) = \frac{1}{2}\left(D(v|G) + \sum_{u\in V(G)} (d(u,v))^2\right),$$

and we call them the *distance number* and the *double distance number* of v, respectively. Then the Wiener and the hyper-Wiener indices can be expressed as:

$$W(G) = \frac{1}{2}\sum_{v\in V(G)} D(v|G),$$

$$WW(G) = \frac{1}{2}\sum_{v\in V(G)} DD(v|G).$$

The Schultz molecular topological index can also be expressed as [5]:

$$MTI(G) = \sum_{v\in V(G)} (d(v))^2 + \sum_{v\in V(G)} d(v)D(v|G).$$

2.1. Theorem. *For $n \geq 5$, let G be a circulant network $C_n(1,2)$. Then*

$$W(G) = \frac{1}{16}\begin{cases} n^2(n+2) & , \text{ when } n \equiv 0,2 \ (mod\ 4),\\ n(n-1)(n+3) & , \text{ when } n \equiv 1 \ (mod\ 4),\\ n(n+1)^2 & , \text{ when } n \equiv 3 \ (mod\ 4).\end{cases}$$

Proof. We discuss the following three cases:
Case 1: When $n \equiv 0,2$ (mod 4). For all $v \in V(G)$, the distance number of v is

$$\begin{aligned} D(v|G) &= \begin{cases} 4(1+2+\ldots+\frac{n-4}{4}) + 3(\frac{n}{4}) & , \text{ when } n \equiv 0 \ (mod\ 4),\\ 4(1+2+\ldots+\frac{n-2}{4}) + 1(\frac{n-2}{4}+1) & , \text{ when } n \equiv 2 \ (mod\ 4),\end{cases}\\ &= \frac{1}{8}n(n+2). \end{aligned}$$

By applying the formula of Wiener index, we have

$$W(G) = \frac{1}{2}\sum_{v\in V(G)} D(v|G) = \frac{1}{2}\sum_{v\in V(G)} \frac{1}{8}n(n+2) = \frac{1}{16}n^2(n+2).$$

Case 2: When $n \equiv 1$ (mod 4). The distance number of each $v \in V(G)$ is

$$D(v|G) = 4\left(1+2+\ldots+\frac{n-1}{4}\right) = \frac{1}{8}(n-1)(n+3).$$

By applying the formula of Wiener index, we have

$$W(G) = \frac{1}{2}\sum_{v\in V(G)} D(v|G) = \frac{1}{2}\sum_{v\in V(G)} \frac{1}{8}(n-1)(n+3) = \frac{1}{16}n(n-1)(n+3).$$

Case 3: When $n \equiv 3 \pmod 4$. The distance number of every vertex v of G is

$$D(v|G) = 4\left(1+2+\ldots+\frac{n-3}{4}\right)+2\left(\frac{n-3}{4}+1\right) = \frac{1}{8}(n+1)^2.$$

By applying the formula of Wiener index, we have

$$W(G) = \frac{1}{2}\sum_{v\in V(G)} D(v|G) = \frac{1}{2}\sum_{v\in V(G)} \frac{1}{8}(n+1)^2 = \frac{1}{16}n(n+1)^2.$$

□

2.2. Theorem. *For $n \geq 5$, let G be a circulant network $C_n(1,2)$. Then*

$$WW(G) = \frac{1}{192}\begin{cases} n^2(n^2+9n+20) & , \ \textit{when } n \equiv 0 \ (mod\ 4), \\ n(n-1)(n+3)(n+7) & , \ \textit{when } n \equiv 1 \ (mod\ 4), \\ n(n+2)(n^2+7n+6) & , \ \textit{when } n \equiv 2 \ (mod\ 4), \\ n(n+1)(n^2+8n+15) & , \ \textit{when } n \equiv 3 \ (mod\ 4). \end{cases}$$

Proof. We discuss the following four cases:
Case 1: When $n \equiv 0 \pmod 4$. For all $v \in V(G)$, the double distance number of v is

$$DD(v|G) = \frac{1}{2}\left(D(v|G) + 4(1^2+2^2+3^2+\ldots+(\frac{n-4}{4})^2) + 3(\frac{n}{4})^2\right).$$

Using the value of $D(v|G)$ derived in Theorem 2.1 (Case-1), we have

$$DD(v|G) = \frac{1}{96}n(n^2+9n+20).$$

By applying the formula of hyper-Wiener index, we have

$$\begin{aligned} WW(G) &= \frac{1}{2}\sum_{v\in V(G)} DD(v|G) \\ &= \frac{1}{2}\sum_{v\in V(G)} \frac{1}{96}n(n^2+9n+20) = \frac{1}{192}n^2(n^2+9n+20). \end{aligned}$$

Case 2: When $n \equiv 1 \pmod 4$. For all $v \in V(G)$, the double distance number of v is

$$DD(v|G) = \frac{1}{2}\left(D(v|G) + 4(1^2+2^2+3^2+\ldots+(\frac{n-1}{4})^2)\right).$$

Using the value of $D(v|G)$ derived in Theorem 2.1 (Case-1), we have

$$DD(v|G) = \frac{1}{96}(n-1)(n+3)(n+7).$$

By applying the formula of hyper-Wiener index, we have

$$\begin{aligned} WW(G) &= \frac{1}{2}\sum_{v\in V(G)} DD(v|G) \\ &= \frac{1}{2}\sum_{v\in V(G)} \frac{1}{96}(n-1)(n+3)(n+7) = \frac{1}{192}n(n-1)(n+3)(n+7). \end{aligned}$$

Case 3: When $n \equiv 2 \pmod 4$. For each vertex v of G, the double distance number of v is

$$DD(v|G) = \frac{1}{2}\left(D(v|G) + 4(1^2+2^2+3^2+\ldots+(\frac{n-2}{4})^2) + 1(\frac{n-2}{4}+1)^2\right).$$

Using the value of $D(v|G)$ derived in Theorem 2.1 (Case-2), we have

$$DD(v|G) = \frac{1}{96}(n+2)(n^2+7n+6).$$

By applying the formula of hyper-Wiener index, we have

$$\begin{aligned} WW(G) &= \frac{1}{2}\sum_{v\in V(G)} DD(v|G) \\ &= \frac{1}{2}\sum_{v\in V(G)} \frac{1}{96}(n+2)(n^2+7n+6) = \frac{1}{192}n(n+2)(n^2+7n+6). \end{aligned}$$

Case 4: When $n \equiv 3 \pmod 4$. For all $v \in V(G)$, the double distance number of v is

$$DD(v|G) = \frac{1}{2}\left(D(v|G) + 4(1^2+2^2+3^2+\ldots+(\frac{n-3}{4})^2) + 2(\frac{n-3}{4}+1)^2\right).$$

Using the value of $D(v|G)$ derived in Theorem 2.1 (Case-3), we have

$$DD(v|G) = \frac{1}{96}(n+1)(n^2+8n+15).$$

By applying the formula of hyper-Wiener index, we have

$$\begin{aligned} WW(G) &= \frac{1}{2}\sum_{v\in V(G)} DD(v|G) \\ &= \frac{1}{2}\sum_{v\in V(G)} \frac{1}{96}(n+1)(n^2+8n+15) = \frac{1}{192}n(n+1)(n^2+8n+15). \end{aligned}$$

□

2.3. Theorem. *For $n \geq 5$, let G be a circulant network $C_n(1,2)$. Then*

$$MTI(G) = \frac{1}{2}n\begin{cases} (n^2+2n+32) & , \text{ when } n \equiv 0,2 \ (mod\ 4), \\ (n^2+2n+29) & , \text{ when } n \equiv 1 \ (mod\ 4), \\ (n^2+2n+33) & , \text{ when } n \equiv 3 \ (mod\ 4). \end{cases}$$

Proof. We discuss the following three cases:

Case 1: When $n \equiv 0,2 \pmod 4$. Since the degree $d(v)$ of each vertex v in G is 4, so using the distance number $D(v|G)$ for each $v \in V(G)$, derived in Theorem 2.1 (Case-1), and by applying the formula of Schultz molecular topological index, we have

$$\begin{aligned} MTI(G) &= \sum_{v\in V(G)} (d(v))^2 + \sum_{v\in V(G)} d(v)D(v|G) \\ &= 16n + 4n\left(\frac{1}{8}n(n+2)\right) = \frac{1}{2}n(n^2+2n+32). \end{aligned}$$

Case 2: When $n \equiv 1 \pmod 4$. Since the degree $d(v)$ of each vertex v in G is 4, so using the distance number $D(v|G)$ for each $v \in V(G)$, derived in Theorem 2.1 (Case-2), and by applying the formula of Schultz molecular topological index, we have

$$\begin{aligned} MTI(G) &= \sum_{v\in V(G)} (d(v))^2 + \sum_{v\in V(G)} d(v)D(v|G) \\ &= 16n + 4n\left(\frac{1}{8}(n-1)(n+3)\right) = \frac{1}{2}n(n^2+2n+29). \end{aligned}$$

Case 3: When $n \equiv 3 \pmod 4$. Since the degree $d(v)$ of each vertex v in G is 4, so using the distance number $D(v|G)$ for each $v \in V(G)$, derived in Theorem 2.1 (Case-3), and by applying the formula of Schultz molecular topological index, we have

$$\begin{aligned} MTI(G) &= \sum_{v\in V(G)} (d(v))^2 + \sum_{v\in V(G)} d(v)D(v|G) \\ &= 16n + 4n\left(\frac{1}{8}(n+1)^2\right) = \frac{1}{2}n(n^2+2n+33). \end{aligned}$$

□

3. Circulant networks $C_n(1,3)$

In this section, we consider circulant networks $C_n(1,3)$, for all $n \geq 7$, in the context of the Wiener, hyper-Wiener and Schultz indices.

3.1. Theorem. *For $n \geq 7$, let G be a circulant network $C_n(1,3)$. Then*

$$W(G) = \frac{1}{24}\begin{cases} n^2(n+8) & , \ when\ n \equiv 0,4\ (mod\ 6), \\ n(n+9)(n-1) & , \ when\ n \equiv 1,3\ (mod\ 6), \\ n(n^2+8n-8) & , \ when\ n \equiv 2\ (mod\ 6), \\ n(n^2+8n+7) & , \ when\ n \equiv 5\ (mod\ 6). \end{cases}$$

Proof. We discuss the following four cases:
Case 1: When $n \equiv 0, 4 \pmod 6$. For all $v \in V(G)$, the distance number of v is

$$\begin{aligned} D(v|G) &= \begin{cases} 4(1) + 6(2+3+\ldots+\frac{n-6}{6}) + 5(\frac{n}{6}) + 2(\frac{n+6}{6}) & , \ n \equiv 0\ (mod\ 6), \\ 4(1+\frac{n+2}{6}) + 6(2+3+\ldots+\frac{n-4}{6}) + 1(\frac{n+8}{6}) & , \ n \equiv 4\ (mod\ 6), \end{cases} \\ &= \frac{1}{12}n(n+8). \end{aligned}$$

By applying the formula of Wiener index, we have

$$W(G) = \frac{1}{2}\sum_{v\in V(G)} D(v|G) = \frac{1}{2}\sum_{v\in V(G)} \frac{1}{12}n(n+8) = \frac{1}{24}n^2(n+8).$$

Case 2: When $n \equiv 1, 3 \pmod 6$. For all $v \in V(G)$, the distance number of v is

$$D(v|G) = \begin{cases} 4(1) + 6(2+3+\ldots+\frac{n-1}{6}) + 2(\frac{n+5}{6})) & , \text{ when } n \equiv 1 \ (mod\ 6), \\ 4(1+\frac{n+3}{6}) + 6(2+3+\ldots+\frac{n-3}{6}) & , \text{ when } n \equiv 3 \ (mod\ 6), \end{cases}$$
$$= \frac{1}{12}(n+9)(n-1).$$

By applying the formula of Wiener index, we have

$$W(G) = \frac{1}{2}\sum_{v\in V(G)} D(v|G) = \frac{1}{2}\sum_{v\in V(G)} \frac{1}{12}(n+9)(n-1) = \frac{1}{24}n(n+9)(n-1).$$

Case 3: When $n \equiv 2$ (mod 6). For all $v \in V(G)$, the distance number of v is

$$D(v|G) = 4(1) + 6(2+3+\ldots+\frac{n-2}{6}) + 3(\frac{n+4}{6})$$
$$= \frac{1}{12}(n^2+8n-8).$$

By applying the formula of Wiener index, we have

$$W(G) = \frac{1}{2}\sum_{v\in V(G)} D(v|G) = \frac{1}{2}\sum_{v\in V(G)} \frac{1}{12}(n^2+8n-8) = \frac{1}{24}n(n^2+8n-8).$$

Case 4: When $n \equiv 5$ (mod 6). For all $v \in V(G)$, the distance number of v is

$$D(v|G) = 4(1+\frac{n+1}{6}) + 6(2+3+\ldots+\frac{n-5}{6}) + 2(\frac{n+7}{6})$$
$$= \frac{1}{12}(n^2+8n+7).$$

By applying the formula of Wiener index, we have

$$W(G) = \frac{1}{2}\sum_{v\in V(G)} D(v|G) = \frac{1}{2}\sum_{v\in V(G)} \frac{1}{12}(n^2+8n+7) = \frac{1}{24}n(n^2+8n+7).$$

□

3.2. Theorem. *For $n \geq 7$, let G be a circulant network $C_n(1,3)$. Then*

$$WW(G) = \frac{1}{432}\begin{cases} n^2(n^2+21n+162) & , \text{ when } n \equiv 0 \ (mod\ 6), \\ n(n^3+21n^2+135n-157) & , \text{ when } n \equiv 1 \ (mod\ 6), \\ n(n^3+12n^2+138n-152) & , \text{ when } n \equiv 2 \ (mod\ 6), \\ n(n^3+21n^2+135n-189) & , \text{ when } n \equiv 3 \ (mod\ 6), \\ n(n^3+21n^2+162n+32) & , \text{ when } n \equiv 4 \ (mod\ 6), \\ n(n^3+21n^2+183n+163) & , \text{ when } n \equiv 5 \ (mod\ 6). \end{cases}$$

Proof. We discuss the following six cases:
Case 1: When $n \equiv 0$ (mod 6). For all $v \in V(G)$, the double distance number of v is

$$DD(v|G) = \frac{1}{2}\left(D(v|G) + 4(1^2) + 6(2^2+\ldots+(\frac{n-6}{6})^2) + 5(\frac{n}{6})^2 + 2(\frac{n+6}{6})^2\right).$$

Using the value of $D(v|G)$ derived in Theorem 3.1 (Case-1), we have

$$DD(v|G) = \frac{1}{216}n(n^2+21n+162).$$

By applying the formula of hyper-Wiener index, we have

$$
\begin{aligned}
WW(G) &= \frac{1}{2}\sum_{v\in V(G)} DD(v|G) \\
&= \frac{1}{2}\sum_{v\in V(G)} \frac{1}{216}n(n^2+21n+162) = \frac{1}{432}n^2(n^2+21n+162).
\end{aligned}
$$

Case 2: When $n \equiv 1 \pmod 6$. For all $v \in V(G)$, the double distance number of v is

$$DD(v|G) = \frac{1}{2}\left(D(v|G) + 4(1^2) + 6(2^2+3^2+\ldots+(\frac{n-1}{6})^2 + 2(\frac{n+5}{6})^2)\right).$$

Using the value of $D(v|G)$ derived in Theorem 3.1 (Case-2), we have

$$DD(v|G) = \frac{1}{216}(n^3+21n^2+135n-157).$$

By applying the formula of hyper-Wiener index, we have

$$
\begin{aligned}
WW(G) &= \frac{1}{2}\sum_{v\in V(G)} DD(v|G) \\
&= \frac{1}{2}\sum_{v\in V(G)} \frac{1}{216}(n^3+21n^2+135n-157) \\
&= \frac{1}{432}n(n^3+21n^2+135n-157).
\end{aligned}
$$

Case 3: When $n \equiv 2 \pmod 6$. For all $v \in V(G)$, the double distance number of v is

$$DD(v|G) = \frac{1}{2}\left(D(v|G) + 4(1^2) + 6(2^2+3^2+\ldots+(\frac{n-2}{6})^2) + 3(\frac{n+4}{6})^2\right).$$

Using the value of $D(v|G)$ derived in Theorem 3.1 (Case-3), we have

$$DD(v|G) = \frac{1}{216}(n^3+21n^2+138n-152).$$

By applying the formula of hyper-Wiener index, we have

$$
\begin{aligned}
WW(G) &= \frac{1}{2}\sum_{v\in V(G)} DD(v|G) \\
&= \frac{1}{2}\sum_{v\in V(G)} \frac{1}{216}(n^3+21n^2+138n-152) \\
&= \frac{1}{432}n(n^3+21n^2+138n-152).
\end{aligned}
$$

Case 4: When $n \equiv 3 \pmod 6$. For all $v \in V(G)$, the double distance number of v is

$$DD(v|G) = \frac{1}{2}\left(D(v|G) + 4(1^2+(\frac{n+3}{6})^2) + 6(2^2+3^2+\ldots+(\frac{n-3}{6})^2)\right).$$

Using the value of $D(v|G)$ derived in Theorem 3.1 (Case-2), we have

$DD(v|G) = \frac{1}{216}(n^3+21n^2+135n-189)$.

By applying the formula of hyper-Wiener index, we have

$$\begin{aligned} WW(G) &= \frac{1}{2}\sum_{v\in V(G)} DD(v|G) \\ &= \frac{1}{2}\sum_{v\in V(G)} \frac{1}{216}(n^3+21n^2+135n-189) \\ &= \frac{1}{432}n(n^3+21n^2+135n-189). \end{aligned}$$

Case 5: When $n \equiv 4 \pmod 6$. For all $v \in V(G)$, the double distance number of v is

$$DD(v|G) = \frac{1}{2}\left(D(v|G) + 4(1^2 + (\frac{n+2}{6})^2) + 6(2^2 + \ldots + (\frac{n-4}{6})^2) + 1(\frac{n+8}{6})^2\right).$$

Using the value of $D(v|G)$ derived in Theorem 3.1 (Case-1), we have

$DD(v|G) = \frac{1}{216}(n^3+21n^2+162n+32)$.

By applying the formula of hyper-Wiener index, we have

$$\begin{aligned} WW(G) &= \frac{1}{2}\sum_{v\in V(G)} DD(v|G) \\ &= \frac{1}{2}\sum_{v\in V(G)} \frac{1}{216}(n^3+21n^2+162n+32) \\ &= \frac{1}{432}n(n^3+21n^2+162n+32). \end{aligned}$$

Case 6: When $n \equiv 5 \pmod 6$. For all $v \in V(G)$, the double distance number of v is

$$DD(v|G) = \frac{1}{2}\left(D(v|G) + 4(1^2 + (\frac{n+1}{6})^2) + 6(2^2 + \ldots + (\frac{n-5}{6})^2) + 2(\frac{n+7}{6})^2\right).$$

Using the value of $D(v|G)$ derived in Theorem 3.1 (Case-4), we have

$DD(v|G) = \frac{1}{216}(n^3+21n^2+183n+163)$.

By applying the formula of hyper-Wiener index, we have

$$\begin{aligned} WW(G) &= \frac{1}{2}\sum_{v\in V(G)} DD(v|G) \\ &= \frac{1}{2}\sum_{v\in V(G)} \frac{1}{216}(n^3+21n^2+183n+163) \\ &= \frac{1}{432}n(n^3+21n^2+183n+163). \end{aligned}$$

□

3.3. Theorem. *For $n \geq 7$, let G be a circulant network $C_n(1,3)$. Then*

$$MTI(G) = \frac{1}{3}n \begin{cases} (n^2+8n+48) & , \quad when\ n \equiv 0,4\ (mod\ 6), \\ (n^2+8n+39) & , \quad when\ n \equiv 1,3\ (mod\ 6), \\ (n^2+8n+40) & , \quad when\ n \equiv 2\ (mod\ 6), \\ (n^2+8n+55) & , \quad when\ n \equiv 5\ (mod\ 6). \end{cases}$$

Proof. We discuss the following four cases:
Case 1: When $n \equiv 0,4$ (mod 6). Since the degree $d(v)$ of each vertex v in G is 4, so using the distance number $D(v|G)$ for each $v \in V(G)$, derived in Theorem 3.1 (Case-1), and by applying the formula of Schultz molecular topological index, we have

$$\begin{aligned} MTI(G) &= \sum_{v\in V(G)} (d(v))^2 + \sum_{v\in V(G)} d(v)D(v|G) \\ &= 16n + 4n\left(\frac{1}{12}n(n+8)\right) = \frac{1}{3}n(n^2+8n+48). \end{aligned}$$

Case 2: When $n \equiv 1,3$ (mod 6). Since the degree $d(v)$ of each vertex v in G is 4, so using the distance number $D(v|G)$ for each $v \in V(G)$, derived in Theorem 3.1 (Case-2), and by applying the formula of Schultz molecular topological index, we have

$$\begin{aligned} MTI(G) &= \sum_{v\in V(G)} (d(v))^2 + \sum_{v\in V(G)} d(v)D(v|G) \\ &= 16n + 4n\left(\frac{1}{12}n(n^2+8n+3)\right) = \frac{1}{3}n(n^2+8n+39). \end{aligned}$$

Case 3: When $n \equiv 2$ (mod 6). Since the degree $d(v)$ of each vertex v in G is 4, so using the distance number $D(v|G)$ for each $v \in V(G)$, derived in Theorem 3.1 (Case-3), and by applying the formula of Schultz molecular topological index, we have

$$\begin{aligned} MTI(G) &= \sum_{v\in V(G)} (d(v))^2 + \sum_{v\in V(G)} d(v)D(v|G) \\ &= 16n + 4n\left(\frac{1}{12}(n^2+8n-8)\right) = \frac{1}{3}n(n^2+8n+40). \end{aligned}$$

Case 4: When $n \equiv 5$ (mod 6). Since the degree $d(v)$ of each vertex v in G is 4, so using the distance number $D(v|G)$ for each $v \in V(G)$, derived in Theorem 3.1 (Case-4), and by applying the formula of Schultz molecular topological index, we have

$$\begin{aligned} MTI(G) &= \sum_{v\in V(G)} (d(v))^2 + \sum_{v\in V(G)} d(v)D(v|G) \\ &= 16n + 4n\left(\frac{1}{12}(n^2+8n+7)\right) = \frac{1}{3}n(n^2+8n+55). \end{aligned}$$

□

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