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Distance in Armchair Polyhex Nanotubes

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Abstract. Topological indices which are derived from the distance matrix of a molecular graph, can be used to characterize aspects of a molecule (e.g. branching) using a single number, derived mathematically in an unambiguous manner from the graph of a molecule. In this paper we give a method to compute the topological indices of $TUVC_6[2p, q]$, the armchair polyhex nanotubes.

1. Introduction

Graph theory is a well-established branch of discrete mathematics and may be applied to chemical problems. In fact a close relationship often exists between the graph of the molecular structures of organic compounds and many of their physical, chemical or biological properties. Particularly interesting are topological indices, derived from the distance matrix of the molecular graph. In a molecular graph, a vertex represents atom and an edge symbolizes bond. Let $G = (V(G), E(G))$ be graph, where $V(G)$ and $E(G)$ are the vertex set and edge set, respectively. If G has n vertices, then the distance matrix, $D = [d(u, v)]_{n\times n}$, is an square symmetric matrix. The entry $d(u, v)$ of matrix D is the length of a shortest path between the vertices u and v in G. In [1] Harold Wiener obtained relations between the half sum of distances between all vertices of the graph of alkanes

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and their physicochemical properties. For an arbitrary connected graph definition of the Wiener index in terms of distances between vertices was the first given by Hosoya in [2]:

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

For a nice survey in this topic we encourage the reader to consult [3]-[5]. The Wiener index has many many generalizations. For example hyper Wiener index, introduced by Klein et al. [6] is defined as

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

(see also [7]-[10].)
Schultz index which is introduced by Schultz in [11], appears to be one of the most studied topological indices. It is defined as

$$S(G) = \sum_{\{u,v\} \subseteq V(G)} (\delta_u + \delta_v) d(u,v),$$

where δ_u is the degree of the vertex u. (see also [12], [13]).
A Wiener index analogue, referred to as the Szeged index, Sz, was recently proposed by Gutman et al. (see for example [14]-[18]). Let u and v be two adjacent vertices of the graph G and $e = uv$ be the edge between them. Let $B_u(e)$ be the set of all vertices of G lying closer to u than to v and $B_v(e)$ be the set of all vertices of G lying closer to v than to u, that is

$$B_u(e) = \{x \mid x \in V(G), d_G(x,u) < d_G(x,v)\}$$
$$B_v(e) = \{x \mid x \in V(G), d_G(x,v) < d_G(x,u)\}.$$

Let $n_u(e) = |B_u(e)|$ and $n_v(e) = |B_v(e)|$. The Szeged index of G is defined as

$$Sz(G) = \sum_{e \in E(G)} n_u(e) n_v(e).$$

Carbon nanotubes were first discovered by Sumio Iijima [19] in 1991 in the deposit formed by the method used for bulk fullerene generation. Since their discovery, they have been the subject of many experimental and theoretical studies owing to their remarkable structural and electronic properties. Topological indices of polyhex nanotoubes have been studied by many of people (see [20]-[29]). In this paper we give a method that enables us to compute different topological indices and polynomials of armchair polyhex nanotubes (see Figure 1), simultaneously.

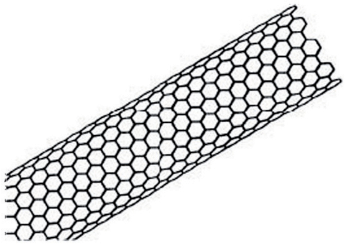

Figure 1: An armchair polyhex nanotube

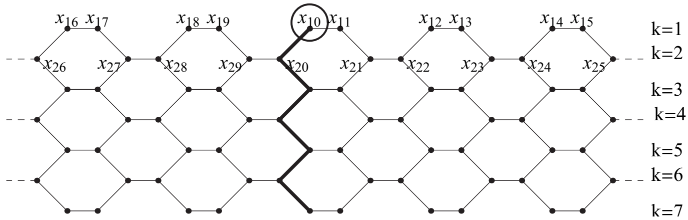

Figure 2: A $TUVC_6[2p, q]$ Lattice with $p = 5$ and $q = 7$.

For this purpose we choose a coordinate label for vertices of $TUVC_6[2p, q]$, armchair polyhex nanotube as shown in Figure 2. Throughout the paper $G := TUVC6[2p, q]$, denotes an arbitrary armchair polyhex nanotube in terms of their circumference $2p$ and their length q.

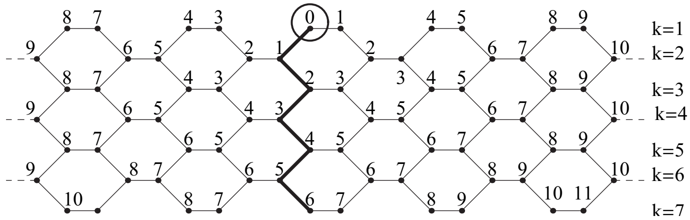

Figure 3: Distances from x_{01} to all vertices of $TUVC_6[2p, q]$ with $p = 5$ and $q = 7$.

2. Primary results on the graph $TUVC_6[2p, q]$

Let λ be a symbol and φ be a function on $A := \{d(u, v) \mid \{u, v\} \subseteq V(G)\}$, where G is a connected graph and $V(G)$ is the set of its vertices. We define $T(G, \lambda)$ as

$$T(G, \lambda) = \sum_{\{u,v\}\subseteq V(G)} \varphi(d(u, v), \lambda).$$

Also for a vertex $u \in V(G)$ we define

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

Then it is easy to see that

$$2T(G, \lambda) = \sum_{u\in V(G)} t(u, \lambda).$$

Firstly we prove the following key lemma:

Lemma 1. In the graph $TUVC_6[2p, q]$ for all vertex u of level 0, the summation $\sum_{x\in \text{ level } k} \varphi(d(u, x), \lambda)$ is constant and is equals to a function of variables p and k. We denote this function by $w(k, p, \lambda)$.

Proof: We calculate the value of $w(k, p, \lambda)$. T first Note that the tube can be built up from two halves collapsing at the polygon line joining x_{10} to $x_{q,0}$ (see Figure 2). The right part is the graph G_1 consists of vertical polygon lines $0, 1, \ldots, p$ and x_{10} is one of the vertices in the first row of the graph G_1. The left part is the graph G_2 consists of vertical polygon lines $(p+1), (p+2), \ldots, 2p-1$. We change the indices of the vertices of G_2 in the following way:

$$V(G_2) = \{\hat{x}_{ji} \mid \hat{x}_{j,i} = x_{j,2p-i} \in V(G)\} \quad \text{(See Figure 3)}$$

We Consider two cases:

Case 1: If $k \geq p$. In the graphs G_1 and for $0 \leq i < k$ we have

$$d(x_{10}, x_{k,i}) = k + i - 1.$$

Also in the graphs G_2 and for $1 \leq i < k$ we have

$$d(x_{10}, \hat{x}_{k,i}) = k + i - 1.$$

So

$$\sum_{x\in \text{ level } k} \varphi(d(x_{10}, x), \lambda) = 2\sum_{i=1}^{p-1} \varphi(k + i - 1, \lambda) + \varphi(0 + k - 1, \lambda) + \varphi(p + k - 1, \lambda).$$

Case 2: $k < p$. First suppose that $1 \leq i < k$. In the graphs G_1 and G_2 we have

$$d(x_{10}, x_{k,i}) = k + i - 1 = d(x_{10}, \hat{x}_{k,i}).$$

We put

$$SS_1 = \sum_{i=0}^{k-1} \varphi(d(x_{10}, x_{k,i}), \lambda) + \sum_{i=1}^{k-1} \varphi(d(x_{10}, \widehat{x}_{k,i}), \lambda).$$

Now suppose that $k \leq i < p$. Then in the graph G_1 we can see that if k is odd, then

$$d(x_{10}, x_{k,i}) = \begin{cases} 2i & \text{if } \ i \ \text{ is even} \\ 2i - 1 & \text{if } \ i \ \text{ is odd} \end{cases}$$

and if k is even, then

$$d(x_{10}, x_{k,i}) = \begin{cases} 2i - 1 & \text{if } \ i \ \text{ is even} \\ 2i & \text{if } \ i \ \text{ is odd.} \end{cases}$$

Also in G_2 we have

$$d(x_{10}, \hat{x}_{k,i}) = \begin{cases} 2i & \text{if } \ i \ \text{ is even} \\ 2i + 1 & \text{if } \ i \ \text{ is odd} \end{cases}$$

if k is odd and

$$d(x_{10}, \hat{x}_{k,i}) = \begin{cases} 2i + 1 & \text{if } \ i \ \text{ is even} \\ 2i & \text{if } \ i \ \text{ is odd} \end{cases}$$

if k is even.
Finally (if $i = p$) in the graph G_1 we have

$$d(x_{10}, x_{k,p}) = H(p, k)$$

where

$$H(p, k) = \begin{cases} 2p - 1 & \text{if } \ k + p \ \text{ is even} \\ 2p & \text{if } \ k + p \ \text{ is odd.} \end{cases}$$

By a straightforward computation we can see

$$\begin{aligned} H(p, k) &= 2p - 1 + irem(k + p, 2) \\ &= 2p - 1 + \frac{1}{2} + \frac{1}{2}(-1)^{k - irem(p,2) + 1}, \end{aligned}$$

where

$$irem(p,2) = \begin{cases} 0 \quad \text{if} \quad p \ \text{ is even} \\ \\ 1 \quad \text{if} \quad p \ \text{ is odd.} \end{cases}$$

We must compute $\sum_{i=k}^{p-1} \varphi(d(x_{10}, x_{ki}), \lambda)$ and $\sum_{i=k}^{p-1} \varphi(d(x_{10}, \widehat{x}_{ki}), \lambda)$. We break down these summations into odd and even indices. Let $A = \{k, k+1, k+2, \ldots, (p-1)\}$, $A_1 = \{i \in A \mid i \text{ is even}\}$ and $A_2 = \{i \in A \mid i \text{ is odd}\}$. Put $S_1 = \sum_{i \in A_1} \varphi(d(x_{10}, x_{ki}), \lambda)$, $S_2 = \sum_{i \in A_2} \varphi(d(x_{10}, x_{ki}), \lambda)$, $\widehat{S}_1 = \sum_{i \in A_1} \varphi(d(x_{10}, \widehat{x}_{ki}), \lambda)$ and $\widehat{S}_2 = \sum_{i \in A_2} \varphi(d(x_{10}, \widehat{x}_{ki}), \lambda)$.

Case 2.1. Suppose that k is odd. Then it is easy to see that

$$\begin{cases} A_1 = \left\{k+2t+1 \mid t = 0, \ldots, \frac{(p-1)-k-1}{2}\right\}, A_2 = \left\{k+2t \mid t = 0, \ldots, \frac{(p-1)-k-1}{2}\right\} & \text{if } p \text{ is odd} \\ \\ A_1 = \left\{k+2t+1 \mid t = 0, \ldots, \frac{(p-1)-k}{2} - 1\right\}, A_2 = \left\{k+2t \mid t = 0, \ldots, \frac{(p-1)-k}{2}\right\} & \text{if } p \text{ is even.} \end{cases}$$

Therefore we have

$$S_1 = \begin{cases} \displaystyle\sum_{t=0}^{\frac{(p-1)-k-1}{2}} \varphi(2(k+2t+1), \lambda) & \text{if } p \text{ is odd} \\ \\ \displaystyle\sum_{t=0}^{\frac{(p-1)-k}{2}-1} \varphi(2(k+2t+1), \lambda) & \text{if } p \text{ is even} \end{cases}$$

and

$$S_2 = \begin{cases} \displaystyle\sum_{t=0}^{\frac{(p-1)-k-1}{2}} \varphi(2(k+2t)-1, \lambda) & \text{if } p \text{ is odd} \\ \\ \displaystyle\sum_{t=0}^{\frac{(p-1)-k}{2}} \varphi(2(k+2t)-1, \lambda) & \text{if } p \text{ is even.} \end{cases}$$

Also we have

$$\widehat{S}_1 = \begin{cases} \displaystyle\sum_{t=0}^{\frac{(p-1)-k-1}{2}} \varphi(2(k+2t+1), \lambda) & \text{if } p \text{ is odd} \\ \\ \displaystyle\sum_{t=0}^{\frac{(p-1)-k}{2}-1} \varphi(2(k+2t+1), \lambda) & \text{if } p \text{ is even} \end{cases}$$

and

$$\widehat{S}_2 = \begin{cases} \displaystyle\sum_{t=0}^{\frac{(p-1)-k-1}{2}} \varphi(2(k+2t)+1,\lambda) & \text{if } p \text{ is odd} \\[2em] \displaystyle\sum_{t=0}^{\frac{(p-1)-k}{2}} \varphi(2(k+2t)+1,\lambda) & \text{if } p \text{ is even.} \end{cases}$$

Therefore the summation of distances from x_{10} to all vertices on level k, in the graph G, is

$$\begin{aligned} \sum_{x\in level\ k} \varphi(d(x_{10},x),\lambda) &= \sum_{i=0}^{k\;\;1} \varphi(d(x_{10},x_{ki}),\lambda) + \sum_{i=1}^{k\;\;1} \varphi(d(x_{10},\widehat{x}_{ki}),\lambda) + \\ & \quad \sum_{i=k}^{p-1} \varphi(d(x_{10},x_{ki}),\lambda) + \sum_{i=k}^{p-1} \varphi(d(x_{10},\widehat{x}_{ki}),\lambda) + \varphi(d(x_{10},x_{kp}),\lambda) \\[1em] &= SS1 + S_1 + S_2 + \widehat{S}_1 + \widehat{S}_2 + \varphi(H(p,k),\lambda) \\ & \qquad\qquad\qquad\qquad \text{(in both cases } p \text{ is odd or even)} \end{aligned}$$

Case 2.2. Suppose that k is even. Then it is easy to see that

$$\begin{cases} A_1 = \left\{k+2t \mid t=0,\dots,\frac{(p-1)-k}{2}\right\}, A_2 = \left\{k+2t+1 \mid t=0,\dots,\frac{(p-1)-k}{2}-1\right\} & \text{if } p \text{ is odd} \\[1.5em] A_1 = \left\{k+2t \mid t=0,\dots,\frac{(p-1)-k-1}{2}\right\}, A_2 = \left\{k+2t+1 \mid t=0,\dots,\frac{(p-1)-k-1}{2}\right\} & \text{if } p \text{ is even.} \end{cases}$$

In this case we put $DS_1 = \sum_{i\in A_1} \varphi(d(x_{10},x_{ki}),\lambda)$, $DS_2 = \sum_{i\in A_2} \varphi(d(x_{10},x_{ki}),\lambda)$, $\widehat{DS}_1 = \sum_{i\in A_1} \varphi(d(x_{10},\widehat{x}_{ki}),\lambda)$ and $\widehat{DS}_2 = \sum_{i\in A_2} \varphi(d(x_{10},\widehat{x}_{ki}),\lambda)$. Therefore

$$DS_1 = \begin{cases} \displaystyle\sum_{t=0}^{\frac{(p-1)-k}{2}} \varphi(2(k+2t)-1,\lambda) & \text{if } p \text{ is odd} \\[2em] \displaystyle\sum_{t=0}^{\frac{(p-1)-k-1}{2}} \varphi(2(k+2t)-1,\lambda) & \text{if } p \text{ is even} \end{cases}$$

and

$$DS_2 = \begin{cases} \displaystyle\sum_{t=0}^{\frac{(p-1)-k}{2}-1} \varphi(2(k+2t+1),\lambda) & \text{if } p \text{ is odd} \\[2em] \displaystyle\sum_{t=0}^{\frac{(p-1)-k-1}{2}} \varphi(2(k+2t+1),\lambda) & \text{if } p \text{ is even.} \end{cases}$$

Also

$$\widehat{DS}_1 = \begin{cases} \displaystyle\sum_{t=0}^{\frac{(p-1)-k}{2}} \varphi(2(k+2t)+1,\lambda) & \text{if } p \text{ is odd} \\ \displaystyle\sum_{t=0}^{\frac{(p-1)-k-1}{2}} \varphi(2(k+2t)+1,\lambda) & \text{if } p \text{ is even} \end{cases}$$

and

$$\widehat{DS}_2 = \begin{cases} \displaystyle\sum_{t=0}^{\frac{(p-1)-k}{2}-1} \varphi(2(k+2t+1),\lambda) & \text{if } p \text{ is odd} \\ \displaystyle\sum_{t=0}^{\frac{(p-1)-k-1}{2}} \varphi(2(k+2t)+1,\lambda) & \text{if } p \text{ is even.} \end{cases}$$

Therefore the summation of distances from x_{10} to all vertices on level k, in the graph G, is

$$\begin{aligned} \sum_{x\in level\ k} \varphi(d(x_{10},x),\lambda) &= \sum_{i=0}^{k-1} \varphi(d(x_{10},x_{ki}),\lambda) + \sum_{i=1}^{k-1} \varphi(d(x_{10},\widehat{x}_{ki}),\lambda) + \\ &\quad \sum_{i=k}^{p-1} \varphi(d(x_{10},x_{ki}),\lambda) + \sum_{i=k}^{p-1} \varphi(d(x_{10},\widehat{x}_{ki}),\lambda) + \varphi(d(x_{10},x_{kp}),\lambda) \\ &= SS1 + DS_1 + DS_2 + \widehat{DS}_1 + \widehat{DS}_2 + \varphi(H(p,k),\lambda) \\ &\qquad\qquad \text{(in both cases } p \text{ is odd or even)} \end{aligned}$$

which, as in the case 2.1, is a function of k and p. □

In the graph G, if we can find a function (for example $w(k,p,\lambda)$ which give us the

$$\sum_{x\in level\ k} \varphi(d(x_{10},x),\lambda),$$

in both cases k is odd or even, then

$$\begin{aligned} t(x_{10},\lambda) &= \sum_{x\in level\ 1} \varphi(d(x_{10},x),\lambda) + \sum_{x\in level\ 2} \varphi(d(x_{10},x),\lambda) + \cdots \\ &+ \sum_{x\in level\ q} \varphi(d(x_{10},x),\lambda) = w(1,p,\lambda) + w(2,p,\lambda) + \cdots + w(q,p,\lambda). \end{aligned}$$

So

$$t(x_{10},\lambda) = t(x_{11},\lambda) = \cdots = t(x_{1,2p-1},\lambda) = w(1,p,\lambda) + w(2,p,\lambda) + \cdots + w(q,p,\lambda). \quad (1)$$

Corollary 2. For each $x_{j,i} \in V(G)$, where $j \geq 2$, we have

$$t(x_{j,i},\lambda) = w(1,p,\lambda) + w(2,p,\lambda) + \cdots + w(q-j+1,p,\lambda) + w(2,p,\lambda) + \cdots + w(j,p,\lambda).$$

Proof: We consider the tube that can be built up from two halves collapsing at level j. The bottom part is the graph $G_1 = TUVC_6[2p, q-j+1]$ and we can consider $x_{j,i}$ as one of the vertices in the first row of the graph G_1. According to (1) we have

$$t_{G_1}(x_{j,i}, \lambda) = w(1, p, \lambda) + w(2, p, \lambda) + \cdots + w(q-j+1, p, \lambda).$$

The top part is the graph $TUVC_6[2p, j] = \widehat{G}_1$ and level j of graph G is the first its row and $x_{j,i}$ is such a vertex of $\widehat{G_1}$. Therefore by (1), $t_{\widehat{G}_1}(x_{j,i}, \lambda) = w(1, p, \lambda) + w(2, p, \lambda) + \cdots + w(j, p, \lambda)$. So

$$\begin{aligned} t_G(x_{j,i}, \lambda) &= t_{G_1}(x_{j,1}, \lambda) + t_{\widehat{G}_1}(x_{j,1}, \lambda) - w(1, p, \lambda) \\ &= w(1, p, \lambda) + w(2, p, \lambda) + \cdots \\ &+ w(q-j+1, p, \lambda) + w(2, p, \lambda) + \cdots + w(j, p, \lambda), \end{aligned}$$

which completes the proof. □

3. Computing $T(G, \lambda)$

The number of vertices and edges of the graph G are $m = 3pq - 2p$ and $n = 2pq$, respectively. We want to determine the sum $\sum\limits_{u \in V(G)} t(u, \lambda)$ that we need to compute $T(G, \lambda)$. For all $1 \leq j \leq q$, put $f(j, \lambda) = t(x_{j,i}, \lambda)$, then by Corollary 2,

$$f(j, \lambda) = \sum_{k=1}^{q-j+1} w(k, p, \lambda) + \sum_{k=2}^{j} w(k, p, \lambda)$$

where $\sum\limits_{k=2}^{1} w(k, p, \lambda) := 0$.

So

$$T(G) = \sum_{j=1}^{q} \sum_{i=0}^{2p-1} t(x_{j,i}, \lambda) = 2p \sum_{j=1}^{q} f(j, \lambda).$$

First suppose that $p \geq q$ and p is even. Then, by the proof of case 2 of Lemma 1, for each $1 \leq k \leq q$ we have

$$w(k, p, \lambda) = SS1 + [S_1 + S_2] + [\widehat{S}_1 + \widehat{S}_2] + \varphi(H(p, k), \lambda)$$

(in both cases p is odd or even).

Therefore we have

$$\begin{aligned} f(j, \lambda) = &\sum_{k=1}^{q-j+1} \Big(SS1 + [S_1 + S_2] + [\widehat{S}_1 + \widehat{S}_2] + \varphi(H(p, k), \lambda) \Big) + \\ &\sum_{k=2}^{j} \Big(SS1 + [S_1 + S_2] + [\widehat{S}_1 + \widehat{S}_2] + \varphi(H(p, k), \lambda) \Big). \end{aligned}$$

Now suppose that $q > p$ and p is even. Let

$$\begin{aligned}
A_1 : &= \{j \mid 1 \le q-j+1 \le p-1, 1 \le j \le p-1\}\\
A_2 : &= \{j \mid 1 \le q-j+1 \le p-1, p \le j \le q\}\\
A_3 : &= \{j \mid p \le q-j+1 \le q, 1 \le j \le p-1\}\\
A_4 : &= \{j \mid p \le q-j+1 \le q, p \le j \le q\}.
\end{aligned}$$

Note that if $A_1 \neq \varnothing$, then $2p-3 \ge q$. Also if $A_4 \neq \varnothing$, then $2p-1 \le q$. Therefore first suppose that $A_1 \neq \varnothing$. Thus $A_4 = \varnothing$ and $2p-3 \ge q$. So,

$$\begin{aligned}
j \in A_1 \implies f(j,\lambda) &= \sum_{k=1}^{q-j+1} \Big(SS1 + [S_1+S_2] + [\widehat{S}_1 + \widehat{S}_2] + \varphi(H(p,k),\lambda)\Big) + \\
&\sum_{k=2}^{j} \Big(SS1 + [S_1+S_2] + [\widehat{S}_1 + \widehat{S}_2] + \varphi(H(p,k),\lambda)\Big).\\
j \in A_2 \implies f(j,\lambda) &= \sum_{k=1}^{q-j+1} \Big(SS1 + [S_1+S_2] + [\widehat{S}_1 + \widehat{S}_2] + \varphi(H(p,k),\lambda)\Big) + \\
&\quad \sum_{k=2}^{p-1} \Big(SS1 + [S_1+S_2] + [\widehat{S}_1 + \widehat{S}_2] + \varphi(H(p,k),\lambda)\Big) + \\
&\quad \sum_{k=p}^{j} \Big(\sum_{i=1}^{p-1} \varphi(k+i-1,\lambda) + \varphi(0+k-1,\lambda) + \varphi(p+k-1,\lambda)\Big).\\
j \in A_3 \implies f(j,\lambda) &= \sum_{k=1}^{p-1} \Big(SS1 + [S_1+S_2] + [\widehat{S}_1 + \widehat{S}_2] + \varphi(H(p,k),\lambda)\Big)\\
&+ \sum_{k=p}^{q-j+1} \Big(\sum_{i=1}^{p-1} \varphi(k+i-1,\lambda) + \varphi(0+k-1,\lambda) + \varphi(p+k-1,\lambda)\Big)\\
&+ \sum_{k=2}^{j} \Big(SS1 + [S_1+S_2] + [\widehat{S}_1 + \widehat{S}_2] + \varphi(H(p,k),\lambda)\Big).
\end{aligned}$$

Since

$$T(G,\lambda) = 2p\sum_{j=1}^{q} f(j,\lambda) \;=\; 2p\Big[\sum_{j\in A_1} f(j,\lambda) + \sum_{j\in A_2} f(j,\lambda) + \sum_{j\in A_3} f(j,\lambda)\Big],$$

So we can compute $T(G,\lambda)$ In this case.

Note that the usefulness of this method depends on we can write the summations

$$SS1 + [S_1+S_2] + [\widehat{S}_1 + \widehat{S}_2] + \varphi(H(p,k),\lambda) \tag{2}$$

$$SS1 + DS_1 + DS_2 + \widehat{DS}_1 + \widehat{DS}_2 + \varphi(H(p,k),\lambda), \tag{3}$$

in fact $w(k,p,\lambda)$, on a function in terms of k and p.

4. Results and Examples

In this section we use the above method to compute the some topological indices of armchair polyhex nanotubes.

Example 1. (See also [23]) Let us compute the Wiener index of $G := TUVC_6[2p,q]$. We define φ,

$$\varphi(d(u,v),\lambda) = d(u,v).$$

Then

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

So the summations (2) and (3) are equal to

$$k^2 + 2p^2 - 2k + \frac{1}{2} + \frac{1}{2}(-1)^{k-irem(p,2)+1}.$$

Therefor

$$w(k,p,\lambda) = \begin{cases} k^2 + 2p^2 - 2k + \frac{1}{2} + \frac{1}{2}(-1)^{k-irem(p,2)+1} & \text{if} \quad 1 \le k < p \\ \\ p(p+2k-2) & \text{if} \quad k \le p. \end{cases}$$

Therefor the Wiener index of $G := TUVC_6[2p,q]$ nanotubes is given by

Case 1: p is even. In this case we have

$$W(G) = \begin{cases} \frac{p}{12}[3(-1)^{q+1} + 3 + 24q^2p^2 - 8q^2 + 2q^4] & \text{if} \quad p > q \\ \\ \frac{-p^2}{6}[8q - 4p + p^3 - 4qp^2 - 4q^3 - 6q^2p] & \text{if} \quad p \le q \end{cases}$$

Case 2: p is odd. In this case we have

$$W(G) = \begin{cases} \frac{p}{12}[3(-1)^{q} - 3 + 24q^2p^2 - 8q^2 + 2q^4] & \text{if} \quad p > q \\ \\ \frac{-p}{6}[-4p63q - 4pq^3 - 6q^2p^2 + 3 + 8qp - 4p^2 + p^4] & \text{if} \quad p \le q \end{cases}$$

Example 2. (See [29]) Now we compute the Szeged index of $G = TUVC_6[2p,q]$. Consider the notations of the above example. We use a theorem of A. Dobrynin and I. Gutman [30] which states that: If G is a connected bipartite graph with n vertices and m edges, then

$$Sz(G) = \frac{1}{4}\Big(n^2m - \sum_{uv\in E(G)} (d(u) - d(v))^2\Big), \tag{4}$$

where for each $v \in V(G)$, $d(v) = \sum_{x \in V(G)} d(v,x)$, is the summation of distances between v and all vertices of G.

Obviously the number of vertices and the number of edges of $G = TUVC_6[2p,q]$ is $n = |V(G)| = 2pq$ and $m = |E(G)| = 3pq - 2p$, respectively. Also G is a bipartite graph. Thus we need to compute $d(u) - d(v)$, for all edges $e = uv$. There are two types of edges in the graph G, horizontal and vertical. In level j for each horizontal for example edge $x_{i,j}x_{i+1,j}$ we have

$$(d(x_{i,j}) - d(x_{i+1,j}))^2 \quad = \quad (f(j,\lambda) - f(j,\lambda))^2 = 0$$

Therefore, we should only calculate for vertical edges. For these vertical vertices it is sufficient calculate for $x_{0,j}x_{0,j+1}$ that $1 \le j \le q-1$. We have

$$d(x_{i,j}) - d(x_{i,j+1}) = d(x_{0,j}) - d(x_{0,j+1}) = f(j,\lambda) - f(j+1,\lambda) = w(q-j+1,p,\lambda) - w(j+1,p,\lambda).$$

Now we are in the position to compute the Szeged index of G.
The Szeged index of $G := TUVC_6[2p,q]$ nanotubes is given by

Case 1: p is even. In this case we have

$$Sz(G) = \begin{cases} \frac{1}{12}p(36p^2q^3 - 24p^2q^2 - 2q^5 - 6q^2 + 6(-1)^q q^2 - 4q^3 + \\ \quad 3q + 6(-1)^{1+q}q + 3(-1)^q q + 6q^4 + 3 + 3(-1)^{1+q}) & \text{if} \quad p \ge q \\ \frac{p}{30}(20q^3p^2 + 4p - 4q - 10p^3 + 6p^5 - q^5 - 30pq^2 + \\ \quad 10pq^4 + 80q^2p^3 + 20p^2q - 40p^4q + 5q^3) & \text{if} \quad 2p > q > p \\ \frac{p^2}{15}(30q^3p - 2 - 13p^4 - 20pq + 15p^2 + 20p^3q) & \text{if} \quad q > 2p \\ \frac{p^2}{15}(267p^4 - 25p^2 - 2) & \text{if} \quad q = 2p \end{cases}$$

Case 2: p is odd. In this case we have

$$Sz(G) = \begin{cases} \frac{1}{12}p(36p^2q^3 - 24p^2q^2 - 2q^5 + 6q^2 + 6(-1)^{-1+q}q^2 - \\ \quad 4q^3 - 9q + 9(-1)^q q + 6q^4 + 3 + 3(-1)^{-1+q}) & \text{if} \quad p \ge q \\ \frac{p}{30}(20q^3p^2 + 4p - 4q - 10p^3 + 6p^5 - q^5 - 30pq^2 + \\ \quad 10pq^4 + 80q^2p^3 + 20p^2q - 40p^4q + 5q^3) & \text{if} \quad 2p > q > p \\ \frac{p^2}{15}(30q^3p - 2 - 13p^4 - 20pq + 15p^2 + 20p^3q) & \text{if} \quad q > 2p \\ \frac{p^2}{15}(267p^4 - 25p^2 - 2) & \text{if} \quad q = 2p \end{cases}$$

Example 3. To compute the Shultz index of $G = TUVC_6[2p, q]$, consider the notations of example 2. Then for $G]$ and for a vertex u of G, $d(u) = \sum_{x \in V(G)} d(u, x)$. Also for each k such that $1 \leq k \leq q$ put $A_k := \{u \in V(G) \mid u \in \ level\ k\}$. Then

$$\begin{aligned}
S(G) &= \sum_{\{u,v\} \subseteq V(G)} (\deg(u) + \deg(v) d(u, v)) \\
&= \frac{1}{2} \sum_{u \in V(G)} \sum_{v \in V(G)} (\deg(u) + \deg(v) d(u, v)) \\
&= \frac{1}{2} \sum_{u \in V(G)} \sum_{v \in V(G)} (\deg(u) d(u, v)) + \frac{1}{2} \sum_{u \in V(G)} \sum_{v \in V(G)} (\deg(v) d(u, v)) \\
&= \frac{1}{2} \sum_{u \in V(G)} \sum_{v \in V(G)} (\deg(u) d(u, v)) + \frac{1}{2} \sum_{v \in V(G)} \sum_{u \in V(G)} (\deg(v) d(u, v)) \\
&= \frac{1}{2} \sum_{u \in V(G)} \deg(u) \sum_{v \in V(G)} d(u, v) + \frac{1}{2} \sum_{v \in V(G)} \deg(v) \sum_{u \in V(G)} d(u, v) \\
&= \frac{1}{2} \sum_{u \in V(G)} \deg(u) d(u) + \frac{1}{2} \sum_{v \in V(G)} \deg(v) d(v) \\
&= \sum_{u \in V(G)} \deg(u) d(u) \\
&= \sum_{u \in V(G) \setminus (A_1 \cup A_q)} \deg(u) d(u) + \sum_{u \in A_1} \deg(u) d(u) + \sum_{u \in A_q} \deg(u) d(u) \\
&= 3[\sum_{u \in V(G)} d(u) - \sum_{u \in A_1} d(u) - \sum_{u \in A_q} d(u)] + 2 \sum_{u \in A_1} d(u) + 2 \sum_{u \in A_q} d(u) \\
&= 6W(G) - [\sum_{u \in A_1} d(u) + \sum_{u \in A_q} d(u)]
\end{aligned}$$

Note that by the definition of φ we have $d(u) = t(u, \lambda)$ so if $u = x_{1,j} \in A_1$, by equation (1) of Lemma 1,

$$d(u) = w(1, p, \lambda) + w(2, p, \lambda) + \cdots + w(q, p, \lambda).$$

Also if $u = x_{q,j} \in A_q$, then by Lemma 2 we have

$$d(u) = w(1, p, \lambda) + w(2, p, \lambda) + \cdots + w(q, p, \lambda).$$

Hence $S(G) = 6W(G) - 4p[w(1, p, \lambda) + w(2, p, \lambda) + \cdots + w(q, p, \lambda)]$.

Example 4. If we define φ ,

$$\varphi(d(u, v), \lambda) = \frac{1}{2}\Big(d(u, v) + d(u, v)^2\Big)$$

then it is easy to see that

$$WW(G) = \sum_{\{u,v\} \subseteq V(G)} \varphi(d(u, v), \lambda).$$

But

$$w(k,p,\lambda) \quad = \quad \begin{cases} -5k^2 + 2p(-1)^{(k-irem(p,2)+1)} + 2p^2 + \frac{8}{3}p^3 + \\ 2k + \frac{1}{3}p + 2k^3 + \frac{1}{2} + \frac{1}{2}(-1)^{(k-irem(p,2)+1)} & \text{if} \quad 1 \leq k < p \\ \\ \frac{1}{3}p[-6k + 1 + 6k^2 - 3p + 6kp + 2p^2] & \text{if} \quad p \leq k. \end{cases}$$

Therefor the hyper Wiener index of $G := TUVC_6[2p,q]$ nanotubes is given by

Case 1: p is even

$$WW(G) = \begin{cases} \frac{p}{120}[48q + 15(-1)^{(q+1)} - 40q^2 + 12q^5 + 120p^2q^2 + 160p^3q^2 + 20pq^2 + \\ \qquad 15 - 60q^3 + 10q^4 + 60p + 60p(-1)^{(q+1)}] & \text{if} \quad p > q \\ \\ \frac{-p^2}{60}[5p^3 - 50p^2 - 20p - 24 + 40q - 30pq^2 - 20p^2q - 50p^3q - 10q^4 - \\ \qquad 20q^3 + 70pq - 20q^3p - 20q^2p^2 + 14p^4] & \text{if} \quad p \leq q \end{cases}$$

Case 2: p is odd

$$WW(G) = \begin{cases} \frac{p}{120}[48q + 15(-1)^q - 40q^2 + 12q^5 + 120p^2q^2 + 160p^3q^2 + 20pq^2 - 15 - \\ \qquad 60q^3 + 10q^4 - 60p + 60p(-1)^q] & \text{if} \quad p > q \\ \\ \frac{-p}{60}[15 + 40pq + 5p^4 - 50p^3 - 20p^2 + 36p - 30q^2p^2 - 20p^3q - 50qp^4 \\ \qquad -10q^4p - 20q^3p + 70p^2q - 20q^3p^2 - 20q^2p^3 + 14p^5] & \text{if} \quad p \leq q. \end{cases}$$

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