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Wiener Index of Armchair Polyhex Nanotubes*

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Formulas for calculating the sum of all distances, known as the Wiener index, in the »armchair« nanotubes are given. The same method was applied in the case of »zig-zag« tubes.

INTRODUCTION

Carbon nanotubes, the one-dimensional carbon allotropes, are intensively studied, with respect to their promise to exhibit unique physical properties: mechanical,[1,2] optical,[3,4] electronic,[5] *etc*. The diameter of single walled nanotubes, SWNTs, is distributed on a large pallet from less than 1 nm to 10 nm or more. Thinner tubes show zero helicity[6] while those with diameters larger than 2 nm usually exhibit defects, kinks, and twists.

Wall defects and open ends may undergo chemical reactions, resulting in functionalized nanotubes.[7] Endohedral functionalization with fullerenes, metals or inorganic salts, penetrating by the capillarity effect the open ends of SWNTs, has also been reported.[8–10]

This paper presents a method for calculating a topological property, namely the sum of all distances, also known as the Wiener index,[11] in »armchair« SWNTs. Note that in the constructive version of Diudea *et al.*,[12–15] this class of non-twisted tubes is named $TUVC_6[c,n]$ (see Figure 1). Wiener index formulas for various classes of tori (*i.e.*, nanotubes the two ends of which are identified) have been presented elsewhere.[16]

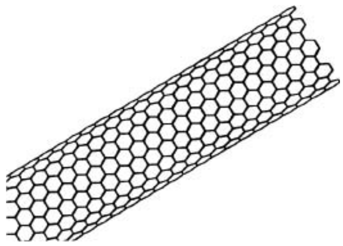

Figure 1. An »armchair« $TUVC_6[20,n]$.

METHOD (A)

Let us consider a hexagonal crenellated (*i.e.*, armchair) lattice, as illustrated in Figure 2. We choose a reference vertex *v*, from which the topological distances to all other vertices are evaluated. The sum of such distances, on each level, is given in the figure as S_i.

* Dedicated to Professor Nenad Trinajstić on the occasion of his 65th birthday for his pioneering activity in Chemical Graph Theory.

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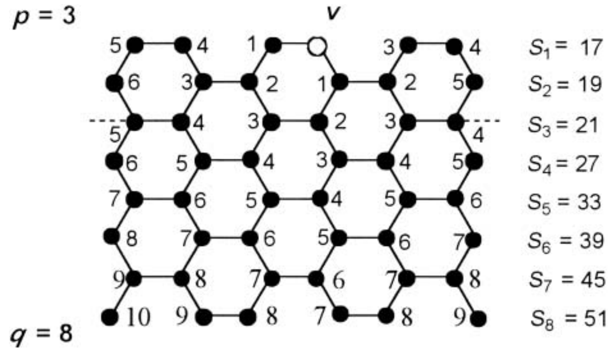

Figure 2. An »armchair« polyhex lattice.

The sum from v to all vertices lying at level $m = 1$ is given by:

$$s_1(p,z) = 2p^2 - z \tag{1}$$

where $z = \mathrm{mod}(p,2)$. Note that in our notation,[12–16] $c = 2p$, $n = q$, and a tube $TUVC_6[c,n]$ is equivalent to a $(c/2, c/2)$ armchair tube.

For levels in the range $1 < k \leq p$, (see the dashed line in Figure 2) the increment to s_1 is calculated as:

$$s_n(k,z) = 2k + 2z - 3 - (-1)^k \tag{2}$$

and the distance sum:

$$s_m(p,s,z) = \sum_{k=1}^{s-z} s_n(k,z) + (2p^2 - z) \tag{3}$$

The total distance sum up to level m is given by:

$$st_m(p,m,z) = (2p^2 - z) + \sum_{s=2}^{m} s_m(p,s,z) \tag{4}$$

The distance sum at level $m = p$ is:

$$s_p(p,z) = \sum_{k=1}^{p-z} s_n(k,z) + (2p^2 - z) \tag{5}$$

Now calculate the sum at levels $m > p$ as:

$$s_c(p,s,z) = s_p(p,z) + 2p(s - p) \tag{6}$$

and the total sum up to m:

$$st_c(p,m,z) = \sum_{s=p+1}^{m} s_c(p,s,z) \tag{7}$$

The total sum from v located at level $m = 1$ to all vertices in $TUVC_6$ will be:

$$s_v(p,m,z) = st_m(p,p,z) + st_c(p,m,z) \tag{8}$$

We are now ready to calculate the Wiener index of a $TUVC_6$ $[2p,q]$ as:

$$W(p,q,z) = \sum_{m=p+1}^{q} 2p \cdot s_v(p,m,z) + \sum_{m=2}^{p} 2p \cdot st_m(p,m,z) + 2p \cdot s_1(p,z) - (q/2) \cdot 2p \cdot s_1(p,z) \tag{9}$$

The subtraction of the last term in the above equation is reasoned as follows: the reference vertex v may be located at any level $1 < m < q$, each time considering TUV as being obtained by two smaller tubes sharing a common level, namely that containing vertex v. It is obvious that the actual level of v is counted twice.

Expansion of functions in (9) leads to the final formula for calculating W, in the case $q \geq p$:

$$W_{TUVC_6}(p,q,z) = \frac{p}{12}\left[\begin{array}{l} 12(-1)^{(p-z)}pq + 3(-1)^{(p-z+1)} + \\ 3(-1)^{-z} - 12q^2z^2 + 12q^2z + \\ 12(-1)^{(p-z)}p + 12z^2q + \\ 6(-1)^{(p-z+1)}p^2 + 8pq^3 - \\ 28pq + 6q^2 + 18q + 8p^3q + \\ 12p^2q^2 - 12(-1)^{(p-z)}q + \\ 6(-1)^{(p-z+1)}q^2 - 24qz - 12p + \\ 14p^2 + 6(-1)^{(1-z)}q - 2p^4 \end{array}\right] \tag{10}$$

Keeping in mind the following:

(i) $(-1)^{(p-z)} = 1$, because:
if p is even, $z = 0$ and $(-1)^{(p-z)} = (-1)^p = 1$
if p is odd, $z = 1$, $p-1$ is even and $(-1)^{(p-z)} = (-1)^{p-1} = 1$

(ii) $(-1)^{(p-z+1)} = (-1) \cdot (-1)^{(p-z)} = (-1)$ since, as calculated above, $(-1)^{p-z} = 1$

(iii) $(-1)^{-z} = (-1)^p$ because:
if p is even and $z = 0$, $(-1)^{-z} = (-1)^0 = 1 = (-1)^p$
if p is odd and $z = 1$, $(-1)^{-z} = (-1)^{-1} = -1 = (-1)^p$

(iv) $z = (1 - (-1)^p) / 2$

relation (10) becomes:

$$W_{TUVC_6}(p,q) = \frac{p}{12} \cdot [p^2(12q^2 - 2p^2 + 8) + 8pq(p^2 + q^2 - 2) + 3(-1 + (-1)^p)] \tag{11}$$

In the case $q \leq p$, (*i.e.*, short tubes, sTUV), W is calculated by the formula:

$$W_{sTUVC_6}(p,q,z) = \sum_{m=2}^{q} 2p \cdot st_m(p,m,z) + 2p \cdot s_1(p,z) - (q/2) \cdot 2p \cdot s_1(p,z) \tag{12}$$

Expansion of functions in (12) leads to the final formula for calculating W, in the case of short tubes:

$$W_{sTUVC_6}(p,q,z) = \frac{p}{12}\left[3(-1)^z + 24p^2q^2 + 2q^4 - 8q^2 + 3(-1)^{(q-z+1)}\right] \tag{13}$$

A similar procedure as used for relation (10) leads to the final formula:

$W_{\mathrm{sTUVC_6}}(p,q) =$

$$\frac{p}{12}\cdot\left[24p^2q^2+2q^4-8q^2+3(-1)^p(1-(-1)^q)\right] \quad (14)$$

For $q = 2$, $p \geq 2$, the formula for simple cycles on $4p$ vertices is recovered:

$$W(C_{4P}) = \frac{p}{4}\left[(-1)^z+32p^2+(-1)^{(1-z)}\right] = 8p^3 \quad (15)$$

METHOD (B)

The sum from v to all vertices lying at level »1« is:

$$s_1(p,z) = 2p_2 - z$$

where $z = \mathrm{mod}(p,2)$.

For levels in the range $1 < k \leq p$, the sum is:

$sv_k(p,k,z) =$

$$2p^2 + z\cdot(-1)^k + (k-1)^2 - \mathrm{mod}((k-1),2) \quad (16)$$

The total distance sum up to level n is given by:

$$st_n(p,n,z) = 2p^2 - z + \sum_{k=2}^{n} sv_k(p,k,z) \quad (17)$$

and, after calculations:

$$st_n(p,n,z) = 2p^2n - \frac{1}{2}\cdot z\cdot[1-(-1)^n] + \frac{1}{3}\cdot n^3 - \frac{1}{2}\cdot n^2 - \frac{1}{3}\cdot n + \frac{1}{4}\cdot[1-(-1)^n] \quad (18)$$

The distance sum at level $n = p$ is:

$$st_p(p) = \frac{7}{3}p^3 - \frac{1}{2}p^2 - \frac{1}{3}p - \frac{1}{4}(1-(-1)^p) \quad (19)$$

Calculate now the sums at levels $k > p$ as follows:

$$svn_p(p,k) = 3p^2 + 2p(k-p-1) \quad (20)$$

The total distance sum from v located at level »1« to all vertices in TUV, for $n > p$, is:

$$stn_p(p,n) = st_p(p) + \sum_{k=p+1}^{n} svn_p(p,k) \quad (21)$$

and, after calculations:

$$stn_p(p,n) = st_p(p) + p(2p+m-1)(m-p) \quad (22)$$

The Wiener index of a $TUVC_6$ $[2p,q]$, $q \geq p$ is given by:

$W_{\mathrm{TUVC_6}}(p,q,z) =$

$$p\cdot\left[2\cdot\sum_{n=1}^{p} st_n(p,n,z) + 2\cdot\sum_{n=p+1}^{q} stn_p(p,n) - q\cdot s_1(p,z)\right] \quad (23)$$

In the case $q \leq p$ (*i.e.*, short tubes, sTUV), the formula is:

$W_{\mathrm{sTUVC_6}}(p,q,z) =$

$$p\cdot\left[2\cdot\sum_{n=1}^{q} st_n(p,n,z) - q\cdot s_1(p,z)\right] \quad (24)$$

Expansion of the above functions leads to the final formulas for calculating W.

Case $q \geq p$ (long tubes, $TUVC_6$):

$W_{\mathrm{TUVC_6}}(p,q,z) =$

$$p\cdot\left[\begin{array}{l}\frac{13}{6}p^4 - \frac{2}{3}p^2 + \frac{(1-2z)}{4}\cdot(1-(-1)^p) + \\ \frac{1}{6}(q-p)[14p^3 + 10p^2\cdot q + 4p\cdot q^2 - \\ 8p - 3 + 3\cdot(-1)^p + 6z \\ \end{array}\right] \quad (25)$$

With $z = (1-(-1)^p)/2$, relation (25) transforms into relation (11).

Case $q \leq p$ (short tubes, sTUV); expansion of relation (24) leads to:

$W_{\mathrm{sTUVC_6}}(p,q,z) =$

$$p\cdot\left[2p^2q^2 + \frac{1}{6}q^4 - \frac{2}{3}q^2 + \frac{1}{4}(1-(-1)^q) - \frac{1}{2}z(1-(-1)^q)\right] \quad (26)$$

Substituting z as above, (26) transforms into relation (14).

Tables I and II list some numerical values for the Wiener index of long $TUVC_6[2p,q]$ and short tubes $sTUVC_6[2p,q]$, respectively.

TABLE I. Wiener index of long tubes, $TUVC_6[2p,q]$, $q \geq p$

p	q	W	p	q	W
3	3	507	4	4	2,176
3	8	5,112	4	8	10,624
3	16	32,136	4	16	62,336
5	5	6,685	6	6	16,704
5	10	32,560	6	12	81,216
5	15	89,685	6	18	223,488
5	20	190,560	6	24	474,624
7	7	36,183	8	8	70,656
7	14	175,784	8	16	343,040
7	21	483,455	8	24	943,104
7	28	1,026,424	8	32	2,001,920

TABLE II. Wiener index of short tubes, sTUVC$_6$[2p,q], $q \leq p$

p	q	W	p	q	W
9	9	127,449	10	10	216,000
9	8	99,072	10	8	134,400
9	7	74,745	10	6	73,920
9	6	54,216	10	5	50,880
9	5	37,233	10	4	32,320
9	4	23,616	10	3	18,080
9	2	5,832	10	2	8,000

METHOD (A). CASE OF »ZIG-ZAG«, TUHC$_6$ [c,n] TUBES

We applied method (A) in the case of »zig-zag«, TUHC$_6$ [2p,q] tubes (Figure 3), as follows:

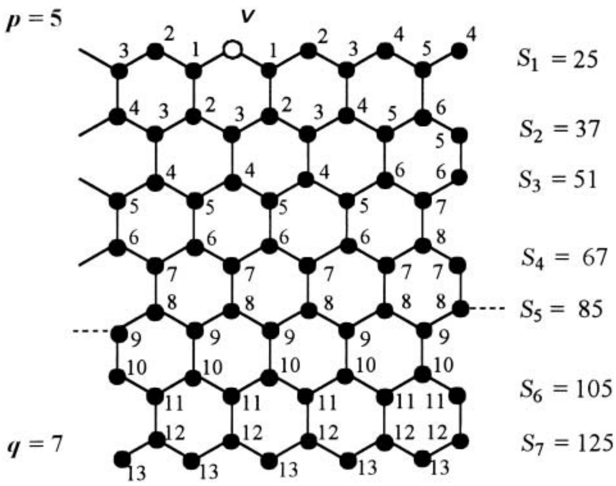

Figure 3. A »zig-zag« polyhex lattice.

The sum from v to all vertices on level m = 1 is:

$$s_1(p,z) = 2p^2 \tag{27}$$

For levels in the range $1 < k \leq p$, the distance sum is now:

$$s_m(p,s) = \sum_{k=1}^{s-1} 2(p+k) + p^2 \tag{28}$$

The total distance sum up to level m is given by:

$$st_m(p,m) = p^2 + \sum_{s=2}^{m} s_m(p,s) \tag{29}$$

The distance sum at level $m = p$ is:

$$s_p(p) = \sum_{k=1}^{p-1} 2(p+k) + p^2 \tag{30}$$

Calculate the sum at levels $m > p$ as:

$$s_c(p,s) = s_p(p) + 4p(s-p) \tag{31}$$

and the total sum up to m:

$$st_c(p,m) = \sum_{s=p+1}^{m} s_c(p,s) \tag{32}$$

The total sum from v located at level m = 1 to all vertices in TUHC$_6$ will be:

$$s_v(p,m) = st_m(p,p) + st_c(p,m) \tag{33}$$

The Wiener index of a TUHC$_6$[2p,q] is now:

$$W(p,q) = \sum_{m=p+1}^{q} 2p \cdot s_v(p,m) + \sum_{m=2}^{p} 2p \cdot st_m(p,m) + 2p \cdot s_1(p,z) - d_a(p) - d_b(p,q) \tag{34}$$

The last two negative terms in the above equation have mainly the same reason as in the case of TUVs and account for the modulo(p,3) and q-dimension, respectively.

The first difference is of the following form:

$$d_a(p) = d_0(p)[(1-\mathrm{mod}(p,3))(2-\mathrm{mod}(p,3)) / 2] + d_1(p)[(2-\mathrm{mod}(p,3))(\mathrm{mod}(p,3))] + d_2(p)[(1-\mathrm{mod}(p,3))(\mathrm{mod}(p,3)) / (-2)] \tag{35}$$

where:

$$d_0(p) = 4p^2 + (\mathrm{trunc}(p/3))(p^3 - p) \tag{36}$$

$$d_1(p) = p^2[4p^2 + (\mathrm{trunc}(p/3))(p+1)] \tag{37}$$

$$d_2(p) = p^2[4p^2 + (1 + \mathrm{trunc}(p/3))(p-1)] \tag{38}$$

Evaluation of $d_a(p)$, in (35) leads to:

$$d_a(p) = (p^2/3)(13p^2 - 1) \tag{39}$$

The second difference $d_b(p,q)$ in (34) is:

$$d_b(p,q) = p^2(q-2p)[4p + (q-2p)] \tag{40}$$

Expansion of all the functions in (34) leads to the final formula for calculating W, in the case of long tubes $q \geq p$:

$$W_{\mathrm{TUHC}_6}(p,q) = \frac{p^2}{6}[8q^3 + 4p^2q - 6q - p^3 + p] \tag{41}$$

which is identical to the formula reported in a preceding paper.[17]

Formula for short tubes (case $q \leq p$, TUHC$_6$), is as follows:

$$W_{\mathrm{sTUHC}_6}(p,q,m) = \sum_{m=2}^{q} 2p \cdot st_m(p,m) + 2p \cdot s_1(p) - (q/2)(2p \cdot s_1(p)) - d_c(p,q) \tag{42}$$

where:

$$d_c(p,q) = p\left(\sum_{k=2}^{q} k(k-1)\right) \tag{43}$$

Expansion of the above functions leads to the final formula for W, in the case of short tubes:

$$W_{\mathrm{sTUHC}_6}(p,q) = \frac{pq}{6}\,[q^3 + 4pq^2 + 6p^2q - q - 4p] \quad (44)$$

For $q = 1$, $p \geq 2$, the formula for simple cycles on $2p$ vertices is recovered:

$$W(C_{2P}) = p^3 \quad (45)$$

CONCLUSIONS

Formulas for calculating the sum of all distances in »armchair« polyhex nanotubes using two methods are given. Method (A) was successfully applied in the case of »zig-zag« tubes.

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SAŽETAK

Wienerov indeks za »armchair« poliheksagonalne nanocijevi

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Dana je formula za izračunavanje Wienerova indeksa za »armchair« poliheksagonalne nanocijevi. Ista je metoda primijenjena i na »zig-zag« poliheksagonalne nanocijevi.