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The Schultz Molecular Topological Index of C_4C_8 Nanotubes[1]

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Abstract

A C_4C_8 net is a trivalent decoration made by alternating squares C_4 and octagons C_8. It can cover either a cylinder or a torus. Such a covering can be derived from a square net by the leapfrog operation. This paper presents a method for calculating the Schultz molecular topological index (MTI) of C_4C_8 nanotubes.

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1 Introduction

Let $G = (V, E)$ be a simple connected graph with the vertex set $V(G)$ and the edge set $E(G)$. For any $i, j \in V(G)$, d_i and D_{ij} denote the degree of i and the distance (i.e., the number of edges on the shortest path) between i and j, respectively.

The Schultz molecular topological index (MTI) of a (chemical) graph G introduced by Schultz [1] in 1989 is defined as

$$MTI = MTI(G) = \sum_{i=1}^{n}\sum_{j=1}^{n} d_i(A_{ij} + D_{ij})$$

where n is the number of vertices of G, $d = (d_1, d_2, \cdots, d_n)$ is the degree vector of vertices of G. A_{ij} is the (i, j)-th entry of the adjacency matrix A of G and A_{ij} is 1 if vertices i and j are adjacent and 0 otherwise.

Let $D_i = \sum_{j=1}^{n} D_{ij}$ be the sum of distances between vertex i and all other vertices. The Schultz molecular topological index can be expressed in the following manner [5]:

$$MTI(G) = \sum_{i=1}^{n} d_i^2 + \sum_{i=1}^{n} d_i D_i \tag{1}$$

The Wiener index $W(G)$ of a connected graph G is equal to the sum of distances between all pairs of vertices of G, i.e.

$$W(G) = \frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n} D_{ij} \tag{2}$$

For details on the Wiener index, which is among the most frequently used molecular-structure-descriptors in chemical graph theory, see the recent survey [2,3].

It has been demonstrated that MTI and W are closely mutually related for certain classes of molecular graphs [4-10]. [10] derived an explicit relation between MTI and W for a tree T with n vertices

$$MTI(T) = 4W(T) + \sum_{i=1}^{n} d_i^2 - n(n-1).$$

Dobrynin [8] gave the explicit relation between the Wiener index and the Schultz molecular topological index of a catacondensed benzenoid graph with h hexagons

$$MTI(G) = 5W(G) - (12h^2 - 14h + 5).$$

Also, [8,9] showed that the Schultz molecular topological index has the same discriminating power with the Wiener index

$$MTI(G_1) = MTI(G_2) \text{ if and only if } W(G_1) = W(G_2)$$

for an arbitrary catacondensed benzenoid graphs.

A C_4C_8 net is a trivalent decoration made by alternating squares C_4 and octagons C_8. It can cover either a cylinder or a torus. Such a covering can be derived from a square net by the leapfrog operation. Let SC_4C_8 and RC_4C_8 denote the C_4C_8 square nanotube and C_4C_8 rhomboidal nanotube, respectively. For the construction of C_4C_8 nanotubes, see [11], where the Wiener indices of SC_4C_8 and RC_4C_8 are computed. The Wiener index and the PI index of tori $T_{p,q}[C_4, C_8]$ and nanotube $SC_4C_8[q, 2p]$ were given in [12-14].

In this paper, we will investigate the relation between the Schultz molecular topological index MTI and the Wiener index W for the C_4C_8 nanotubes, and calculate the Schultz molecular topological index of C_4C_8 nanotubes by the Wiener index of C_4C_8 nanotubes.

2 The Schultz molecular topological index of C_4C_8 square nanotubes

Note that the degrees of vertices in an arbitrary C_4C_8 nanotube G are two or three. The Wiener index $W(G)$ can be written as

$$W(G) = \frac{1}{2}(W_2(G) + W_3(G)),$$

where $W_2(G) = \sum_{d_i=2} D_i$ and $W_3(G) = \sum_{d_i=3} D_i$, the summation $\sum_{d_i=k}$ goes over all vertices of G with degree k.

Let $G = SC_4C_8[p, q]$ be the C_4C_8 square nanotube with p squares at each level and q levels (see Figure 1). Then the Wiener index of G was given in [11]:

Lemma 1([11]). The Wiener index of the nanotube $G = SC_4C_8(S)[p, q]$ is

$$W(G) = \begin{cases} \frac{2}{3}pq(q+1)(q^2+4pq-4p-q+12p^2) - 8p^3q, & 1 \le q \le p+1; \\ \frac{2}{3}p^2(8q^3 - p^3 + 4p^2q + 6pq^2 + p - 6q, & q \ge p+2. \end{cases}$$

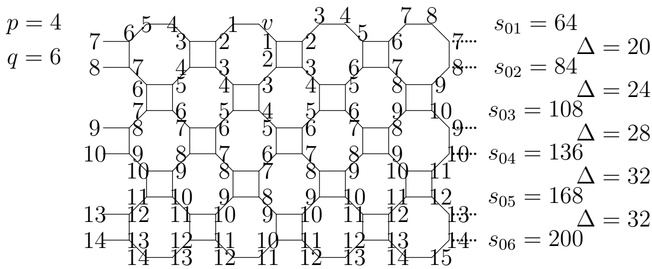

Figure 1. The distance sums from the vertex v to the vertices at levels $k = 1, 2, \cdots, 6$.

Now, we derive a formula for calculating the Schultz molecular topological index of $SC_4C_8[p, q]$ nanotube.

Note that the numbers of vertices with degree 2 and 3 in the graph $G = SC_4C_8[p, q]$ are $4p$ and $4p(q-1)$, respectively. The equation (1) can be further expressed as:

$$\begin{aligned} MTI(G) &= \sum_{i=1}^{n} d_i^2 + \sum_{i=1}^{n} d_i D_i \\ &= 4 \cdot 4p + 9 \cdot 4p(q-1) + 6W(G) - \sum_{d_i=2} D_i \\ &= 6W(G) + 36pq - 20p - W_2(G) \end{aligned} \tag{3}$$

Let $s_{0k} = \sum_{x \text{ is at level } k} D_{vx}$ be the sum of distances from v to all other vertices at level k, where v is a vertex of degree 2 at level 1 (see Figure 1). By the symmetry of G, $W_2(G) = 4p \sum_{k=1}^{q} s_{0k}$.

From [11,14], we know that

$$s_{0k} = \begin{cases} 4p^2 + 2(k-1)(2p+k), & 1 \le k \le p+1; \\ s_{0,p+1} + 8p(k-p-1) = 2p^2 - 6p + 8pk, & p+2 \le k \le q. \end{cases}$$

So,

$$W_2(G) = \begin{cases} -\frac{8}{3}pq - 8p^2q + 16p^3q + 8p^2q^2 + \frac{8}{3}pq^3, & 1 \le q \le p+1; \\ -\frac{8}{3}p^2 + \frac{8}{3}p^4 - 8p^2q + 8p^3q + 16p^2q^2, & q \ge p+2. \end{cases}$$

Combining the equation (3) with Lemma 1, we have

Theorem 2. The Schultz molecular topological index $MTI(G)$ of the nanotube $G = SC_4C_8[p, q]$ is

(i) $-20p + \frac{260}{3}pq - 8p^2q - 64p^3q + 44pq^2 - 8p^2q^2 - \frac{8}{3}pq^3 + 16p^2q^3 + 4pq^4$, for $1 \le q \le p+1$;

(ii) $-20p+\frac{8}{3}p^2+4p^3-\frac{8}{3}p^4-4p^5+36pq-16p^2q-8p^3q+16p^4q-16p^2q^2+24p^3q^2+32p^2q^3$, for $q \geq p+2$.

3 The Schultz molecular topological index of C_4C_8 rhomboidal nanotubes

Let $G = RC_4C_8[p, q]$ be the C_4C_8 rhomboidal nanotube with p rhombuses at each level and q levels (see Figure 2). Then the Wiener index of G was given in [11]:

Lemma 3([11]). The Wiener index $W(G)$ of the nanotube $G = RC_4C_8[p, q]$ is

(i)$\frac{1}{6}pq(16q^3 + 16pq^2 + 36p^2q + 3q(-1)^p - 7q - 6p)$, for $1 \leq q \leq int[\frac{(p+1)}{2}]$;

(ii)$-\frac{1}{24}p[4p^4 - 48p^2q^2 - 192pq^3 - 32p^3q + 24q^2[1-(-1)^p] - p^2 - 3p^2(-1)^p + 68pq + 12pq(-1)^p - 3[1-(-1)^p]]$, for $q \geq int[\frac{(p+1)}{2}] + 1$,
where $int[x]$ is the greatest integer no more than x. i.e.,

(i)$\frac{1}{6}pq(16q^3 + 16pq^2 + 36p^2q - 4q - 6p)$, for $1 \leq q \leq \frac{p}{2}$ and p is even;

(ii)$\frac{1}{6}pq(16q^3 + 16pq^2 + 36p^2q - 10q - 6p)$, for $1 \leq q \leq \frac{p+1}{2}$ and p is odd;

(iii)$-\frac{1}{24}p(4p^4 - 48p^2q^2 - 192pq^3 - 32p^3q - 4p^2 + 80pq)$, for $q \geq \frac{p}{2} + 1$ and p is even;

(iv)$-\frac{1}{24}p(4p^4 - 48p^2q^2 - 192pq^3 - 32p^3q + 48q^2 + 2p^2 + 56pq - 6)$, for $q \geq \frac{p+1}{2} + 1$ and p is odd.

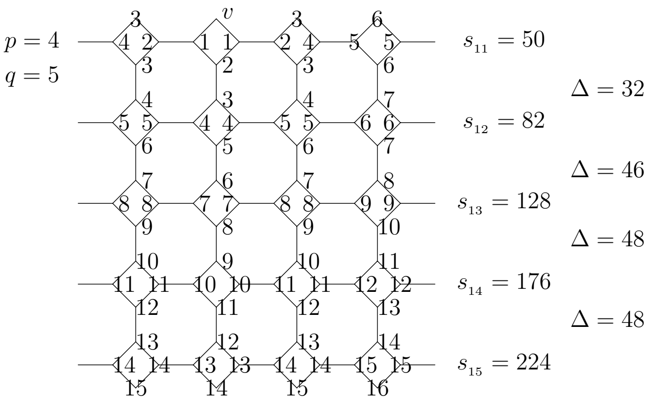

Figure 2. Distance sums from the vertex v to vertices at levels $k = 1, 2, \cdots, 5$.

As in the section two, we derive a formula for calculating the Schultz molecular topological index of $RC_4C_8[p, q]$ nanotube.

Note that the numbers of vertices with degree 2 and 3 in the graph $G = RC_4C_8$ are $2p$ and $2p(2q-1)$, respectively. The equation (1) can be further expressed as:

$$MTI(G) = \sum_{i=1}^{n} d_i^2 + \sum_{i=1}^{n} d_i D_i = 6W(G) + 36pq - 10p - W_2(G) \qquad (4)$$

Let $s_{1k} = \sum_{x \text{ is at level } k} D_{vx}$ be the sum of distances from v to all other vertices at level k, where v is a vertex of degree 2 at level 1 (see Figure 2). By the symmetry of G,

$$W_2(G) = 2p \sum_{k=1}^{q} s_{1k}. \qquad (5)$$

And

$$s_{1k} = \begin{cases} 3p^2 + 2 + 4(k-1)(2k+p), & 1 \le k \le \frac{p}{2} \text{ and } p \text{ is even;} \\ 3p^2 + 1 + 4(k-1)(2k+p), & 1 \le k \le \frac{p+1}{2} \text{ and } p \text{ is odd.} \end{cases}$$

$$\begin{aligned} s_{1k} &= \begin{cases} s_{1,\frac{p}{2}} + 12(p-1) + 10, & k = \frac{p}{2} + 1 \text{ and } p \text{ is even;} \\ s_{1,\frac{p}{2}+1} + 12p(k - \frac{p}{2} - 1), & k \ge \frac{p}{2} + 2 \text{ and } p \text{ is even;} \\ s_{1,\frac{p+1}{2}} + 12p(k - \frac{p+1}{2}), & k \ge \frac{p+1}{2} + 1 \text{ and } p \text{ is odd;} \end{cases} \\ &= \begin{cases} p^2 + 12pk - 8p, & k \ge \frac{p}{2} + 1 \text{ and } p \text{ is even;} \\ p^2 + 12pk - 8p - 1, & k \ge \frac{p+1}{2} + 1 \text{ and } p \text{ is odd.} \end{cases} \end{aligned}$$

From (5), we have

(i) If p is even and $1 \le q \le \frac{p}{2}$, then

$$W_2(G) = -\frac{4}{3}pq - 4p^2q + 6p^3q + 4p^2q^2 + \frac{16}{3}pq^3;$$

(ii) If p is even and $q \ge \frac{p}{2} + 1$, then

$$W_2(G) = -\frac{2}{3}p^2 + \frac{2}{3}p^4 - 4p^2q + 2p^3q + 12p^2q^2;$$

(iii) If p is odd and $1 \le q \le \frac{p+1}{2}$, then

$$W_2(G) = -\frac{10}{3}pq - 4p^2q + 6p^3q + 4p^2q^2 + \frac{16}{3}pq^3;$$

(iv) If p is odd and $q \ge \frac{p+1}{2} + 1$, then

$$W_2(G) = -\frac{2}{3}p^2 + \frac{2}{3}p^4 - 2pq - 4p^2q + 2p^3q + 12p^2q^2.$$

Combining the equation (4) and Lemma 3, we have

Theorem 4. The Schultz molecular topological index $MTI(G)$ of the nanotube $G = RC_4C_8[p,q]$ is

(i)$-10p + \frac{112}{3}pq - 2p^2q - 6p^3q - 4pq^2 - 4p^2q^2 + 36p^3q^2 - \frac{16}{3}pq^3 + 16p^2q^3 + 16pq^4$ for $1 \le q \le \frac{p}{2}$ and p is even;

(ii)$-10p + \frac{118}{3}pq - 2p^2q - 6p^3q - 10pq^2 - 4p^2q^2 + 36p^3q^2 - \frac{16}{3}pq^3 + 16p^2q^3 + 16pq^4$ for $1 \le q \le \frac{p+1}{2}$ and p is odd;

(iii)$-10p + \frac{2}{3}p^2 + p^3 - \frac{2}{3}p^4 - p^5 + 36pq - 16p^2q - 2p^3q + 8p^4q - 12p^2q^2 + 12p^3q^2 + 48p^2q^3$ for $q \ge \frac{p}{2} + 1$ and p is even;

(iv)$-\frac{17}{2}p + \frac{2}{3}p^2 - \frac{1}{2}p^3 - \frac{2}{3}p^4 - p^5 + 38pq - 10p^2q - 2p^3q + 8p^4q - 12pq^2 - 12p^2q^2 + 12p^3q^2 + 48p^2q^3$ for $q \ge \frac{p+1}{2} + 1$ and p is odd.

References

[1] H.P.Schultz, Topological Organic Chemistry. 1. Graph Theory and Topological Indices of Alkanes, *J. Chem. Inf. Comput. Sci. 29*, (1989), 227-228.

[2] A.A.Dobrynin, R.Entringer, I.Gutman, Wiener index of trees: theory and applications, *Acta Appl. Math. 66*, (2001), 211-249.

[3] A.A.Dobrynin, I.Gutman, S.Klavžar, P.Žigert, Wiener index of hexagonal systems, *Acta Appl. Math. 72*, (2002), 247 - 294.

[4] I.Gutman, S. Klavžar, Bounds for the Schultz molecular topological index of benzenoid systems in terms of the Wiener index, *J. Chem. Inf. Comput. Sci. 37*, (1997), 741-744.

[5] S.Klavžar, I.Gutman, A comparison of the Schultz molecular topological index with the Wiener index, *J. Chem. Inf. Comput. Sci. 36*, (1996), 1001-1003.

[6] I.Gutman, Selected properties of the Schultz molecular topological index, *J. Chem. Inf. Comput. Sci. 34*, (1994), 1087-1089.

[7] D.Plavšić, S.Nikolić, N.Trinajstić, D.J.Klein, Relaton between the Wiener index and the Schultz index for several classes of chemical graphs, *Croat. Chem. Acta 66*, (1993), 345-353.

[8] A.A.Dobrynin, Explicit relation between the Wiener index and the Schultz index of catacondensed benzenoid graphs, *Croat. Chem. Acta 72*, (1999), 869-874.

[9] A.A.Dobrynin, Discriminating power of the Schultz index for catacondensed benzenoid graphs, *MATCH Commun. Math. Comput. Chem. 38*, (1998), 19-35.

[10] D.Klein, Z.Mihalić, D.Plavšić, N.Trinajstić, Molecular topological index: a relation with the Wiener index, *J. Chem. Inf. Comput. Sci. 32*, (1992), 304-305.

[11] M.Stefu, M.V.Diudea, Wiener index of C_4C_8 nanotubes, *MATCH Commun. Math. Comput. Chem. 50*, (2004), 133-144.

[12] H.Deng, Wiener index of Tori $T_{p,q}[C_4, C_8]$ covered by C_4 and C_8, *MATCH Commun. Math. Comput. Chem. 56*,(2006), 357-374.

[13] H.Deng, J.Hou, PI indices of nanotubes $SC_4C_8[q, 2p]$ covering by C_4 and C_8, *MATCH Commun. Math. Comput. Chem. 57*, (2007), 503-516.

[14] L.Xu, H.Deng, PI indices of tori $T_{p,q}[C4, C8]$ covered by C_4 and C_8, *MATCH Commun. Math. Comput. Chem. 57*, (2007), 485-502.