Digest Journal of Nanomaterials and Biostructures Vol. 4, No.3, September 2009, p. 453-457

THE HOSOYA POLYNOMIAL OF $TUC_4C_8(S)$ NANOTUBES

ALI REZA ASHRAFI, HOSEIN SHABANI
Institute of Nanoscience and Nanotechnology, University of Kashan,
Kashan 87317-51167, Iran

The Hosoya polynomial of a molecular graph G is defined as $H(G,x) = \sum_{\{u,v\}\subseteq V(G)} x^{d(u,v)}$, where the sum is over all unordered pairs {u,v} of distinct vertices in G. The aim of this paper is to present a new algorithm for computing Hosoya polynomial of $TUC_4C_8(S)$ nanotubes.

(Received June 5, 2008; accepted July 9, 2009)

Keywords: $TUC_4C_8(S)$ nanotube, Hosoya polynomial

1. Introduction

One of the main distinctive characteristics of modern chemistry is the use of theoretical tools for the molecular modeling of physicochemical processes, chemical reaction, medicinal and toxicological events, etc., in which chemicals are involved. Topological indices are one of the main theoretical tools for studying molecular properties of chemical compounds. Here, a topological index is a real number that is derived from molecular graphs of chemical compounds. Such numbers based on the distances in a graph are widely used for establishing relationships between the structure of molecules and their physico-chemical properties. It is easy to see that the number of atoms and the number of bonds in a molecular graph are topological index. The first non trivial topological index was introduced early by Wiener.[1] He defined his index as the sum of distances between any two carbon atoms in the molecules, in terms of carbon-carbon bonds. We encourage the reader to consult papers[2,3] and references therein, for further study on the topic.

Let G be a simple molecular graph without directed and multiple edges and without loops, the vertex and edge sets of which are represented by V(G) and E(G), respectively. If e is an edge of G, connecting the vertices u and v then we write e = uv. The distance between a pair of vertices u and v of G is denoted by d(u,w). Thus, we can redefine the Wiener index of a graph G as $W(G) = \sum_{\{x,y\}\subseteq V(G)} d(x,y)$.

The Hosoya polynomial of a molecular graph G is defined as $H(G,x) = \sum_{\{u,v\}\subseteq V(G)} x^{d(u,v)}$, where the sum is over all unordered pairs {u,v} of distinct vertices in G.[4,5] Suppose $D = [d_{ij}]$ denotes the distance matrix of G, where d_{ij} is the length of a minimal path connecting the ith and jth vertices of G. Then one can see that $W(G) = 1/2\sum_{i,j} d_{ij}$ and $H(G,x) = 1/2\sum_{i,j} x^{d_{ij}}$.

Diudea and his co-authors[6-9] was the first scientist considered topological indices of nanostructures into account. In some research paper, he and his team computed the Wiener index of armchair, zig-zag and $TUC_4C_8(R/S)$ nanotubes. One of us (ARA) continued this program to compute the Wiener index of a polyhex and $TUC_4C_8(R/S)$ nanotori.[10-15] In this paper we continue this program to compute the Hosoya polynomial of a $TUC_4C_8(S)$ nanotube. Our notation is standard and mainly taken from the book of Trinajestic[16] and papers by Taeri and his co-authors.[17-19].

2. Results

In this section an exact formula for the Hosoya polynomials of $TUC_4C_8(S)$ nanotubes are derived, Figure 1. Since $d/dx(W(G,x))|_{x=1}=W(G)$, the Wiener index of these nanomaterials are also computed.

Suppose T is 2–dimensional lattice of $TUC_4C_8(S)[m,n]$, where m is the number of rows and n is the number of columns. Choose eight base vertices $x_k(1,1)$, $x_k\in\{a_1, b_1, c_1, d_1, a_2, b_2, c_2, d_2\}$, Figure 2. We partition V(T) into eight parts as $P = \{A_1, A_2, B_1, B_2, C_1, C_2, D_1, D_2\}$ where $X_j\in P$ and $X_j = \{x_k(i,t): 1 \le i \le m, 1 \le t \le n, k = j\}$. To compute D(T), we must calculate matrices $D^{X_j}_{x_k(1,1)}$. For example $D^{A_1}_{a_1(1,1)}$ is a matrix in which its entries are the distances from $a_1(1,1)$ to all of vertexes A_1. The first row of D(T) is the all entries of eight matrices of vertex $a_1(1,1)$, and other rows are obtained similarly. We notice that making use of symmetry in T, we don't need to investigate the vertices with subscript 2. This fact has been shown in Figure 2. Hence the computation of sixty four matrices presented above, decreases to thirty two matrices.

If we show this matrix by $D^{X_j}_{x_k(1,1)} = \left[(X_j^{x_k})_i\right]_{1\le i\le m}$ where $(X_j^{x_k})_i$ is i^{th} row of the matrix and $k\in\{1,2\}$. We can obtain other matrices for the t^{th} row $(2 \le t \le m)$ and first column of T. For instance, we consider the case of $a_1(t,1)$. Then,

$$D^{A_1}_{a_1(t,1)} = \begin{bmatrix} (A_1^{a_1})_t \\ \vdots \\ (A_1^{a_1})_2 \\ (A_1^{a_1})_1 \\ \vdots \\ (A_1^{a_1})_{m-t+1} \end{bmatrix} \quad \text{and} \quad D^{B_1}_{a_1(t,1)} = \begin{bmatrix} (D_1^{c_1})_t \\ \vdots \\ (D_1^{c_1})_2 \\ (A_1^{b_1})_1 \\ \vdots \\ (A_1^{b_1})_{m-t+1} \end{bmatrix}.$$

Similarly we acquire other matrices of the first column. Notice that finding the matrices of other columns are the same and is omitted. Now we enumerate the entries of distance matrix D(T). Define α_i, $(1 \le i \le m)$, by

$$\alpha_i = \begin{pmatrix} 1 & 2 & \dots & i & i+1 & \dots & m \\ i & i-1 & \dots & 1 & 2 & \dots & m-i+1 \end{pmatrix},$$

Then we can see that the times of repeating s^{th} row matrix $D^{X_j}_{x_1(1,1)}$ is the number of columns in T multiplied by the number of members of the set $\{\alpha_j(j+s-1), \alpha_j(j-s+1) : j, j+s-1, j-s+1 \le m\}$. Consequently, for $D^{X_j}_{x_1(1,1)}$ we obtain the following polynomial:

$$W^{X_j}_{x_k(1,1)}(T,x) = \frac{1}{2}\times 2n\left[\left(m\sum_{j=1}^{n} x^{d_{1j}}\right) + \left(\sum_{i=2}^{m} 2(m-i+1)\left(\sum_{j=1}^{n} x^{d_{ij}}\right)\right)\right]$$

So the Wiener polynomial of T is $W(T,x) = \sum_{X_j,x_1} W^{X_j}_{x_1(1,1)}(T,x)$.

Table 1. $D^{A_1}_{a_1(1,1)} = [d_{ij}]$

$i = 1$	$j = 1$	$2 \le j \le n/2+1$ $(n \mid 2)$ $2 \le j \le (n+1)/2$ $(n \nmid 2)$	$i > 1$	$1 \le j \le n/2+1$ $(n \mid 2)$ $1 \le j \le (n+1)/2$ $(n \nmid 2)$
	$d_{11}=0$	$d_{ij} = d_{1(j-1)} + 4$		$i \le j$ $\quad d_{ij} = d_{(i-1)j} + 2$ $i > j$ $\quad d_{ij} = d_{(i-1)j} + 4$
$d_{ij} = d_{i(n-j+2)}$ where $[n/2+1 < j \le n \;\&\; (n \mid 2)]$ or $[(n+1)/2 < j \le n \;\&\; (n \nmid 2)]$				

- It is clear that three matrices $D^{B_1}_{b_1(1,1)}$, $D^{B_1}_{c_1(1,1)}$ and $D^{D_1}_{d_1(1,1)}$ are equal to $D^{A_1}_{a_1(1,1)}$.
- If we add one to all entries of $D^{A_1}_{a_1(1,1)}$, we obtain $D^{C_1}_{b_1(1,1)}$.
- The rows from two to m of $D^{A_1}_{d_1(1,1)}$, are equal to the rows from one to $(m-1)$ of $D^{A_1}_{a_1(1,1)}$.

Moreover, the first and the second row are equal, except the first entry of first row which is equal to 3.

-

Table 2. $D^{B_1}_{a_1(1,1)} = [s_{ij}]$.

$i = 1$	$j = 1$	$j = 2$	$2 \le j \le n/2+1$ $(n \mid 2)$ $2 \le j \le (n+1)/2+1$ $(n \nmid 2)$	$i > 1$	$j = 1$	$2 \le j \le n/2+1$ $(n \mid 2)$ $2 \le j \le (n+1)/2+1$ $(n \nmid 2)$
	$s_{11} = 1$	$s_{12} = 3$	$s_{1j} = s_{1(j-1)} + 4$		$s_{i1} = s_{(i-1)1} + 4$	$i-1 \le j$ $\quad s_{ij} = s_{(i-1)j} + 2$ $i-1 > j$ $\quad s_{ij} = s_{(i-1)j} + 4$
Then $s_{ij} = s_{i(n-j+3)}$ where $[n/2+1 < j \le n \;\&\; (n \mid 2)]$ or $[(n+1)/2 < j \le n \;\&\; (n \nmid 2)]$						

- Adding one to all entries $D^{B_1}_{a_1(1,1)}$, we obtain $D^{C_1}_{a_1(1,1)}$.
- The first and second row of $D^{B_1}_{d_1(1,1)}$ are equal; also the rows from two to m are equal to the rows from one to $(m-1)$ of $D^{B_1}_{a_1(1,1)}$.
- The first row of $D^{C_1}_{d_1(1,1)}$ and the first row of $D^{B_1}_{a_1(1,1)}$ are the same; the second until m^{th} rows of this matrix, obtained by adding the number two to all entries of the rows from one to $(m-1)$ of $D^{B_1}_{a_1(1,1)}$.
- For columns $1 \le j \le n/2+1$ (n is even) or $1 \le j \le (n+1)/2$ (n is odd), we add entries of $D^{B_1}_{a_1(1,1)}$ by 2. Then for $n/2+1 < j \le n$ (n is even) or $(n+1)/2 < j \le n$ (n is odd) we define $v_{ij} = v_{i(n-j+2)}$ and so $D^{D_1}_{a_1(1,1)} = [v_{ij}]$.
- The rows from two to m of $D^{B_1}_{c_1(1,1)}$ are equal to the rows from one to $(m-1)$ of $D^{D_1}_{a_1(1,1)}$; and the first entry of the first row is one and remaining entries are equal to the second row.
- For columns $1 \le j \le n/2$ (n is even) or $1 \le j \le (n+1)/2$ (n is odd), we add one to the entries of $D^{D_1}_{a_1(1,1)}$ and for columns $n/2 < j \le n$ (n is even) or $(n+1)/2 < j \le n$ (n is odd) we add -1 ot the entries of $D^{D_1}_{a_1(1,1)}$ to obtain $D^{D_2}_{a_1(1,1)}$.
- The first and second rows of $D^{B_2}_{c_1(1,1)} = [w_{ij}]$ are equal, except the last entry of the first row which is equal to 2; and the rows from two to m are got by the equation $w_{ij} = s_{(i-1)(n-j+1)}$.

Table 3. $D^{A_2}_{a_1(1,1)} = [r_{ij}]$

$i = 1$	$j = 1$	$j = n$	$2 \le j \le n/2$ $(n\vert 2)$ $2 \le j \le (n+1)/2$ $(n\nmid 2)$	$n/2 < j < n$ $(n\vert 2)$ $(n+1)/2 < j < n$ $(n\nmid 2)$
	$r_{11} = 1$	$r_{1n} = 3$	$r_{1j} = r_{1(j-1)} + 4$	$r_{1j} = r_{1(j+1)} + 4$
$i > 1$	$1 \le j \le n/2$ $(n\vert 2)$ $1 \le j \le (n+1)/2$ $(n\nmid 2)$			$n/2+1 \le j \le n$ $(n\vert 2)$ $(n+1)/2+1 \le j \le n$ $(n\nmid 2)$
	$i \le j$ $r_{ij} = r_{(i-1)j} + 2$ $i > j$ $r_{ij} = r_{(i-1)j} + 4$			$i \le n-j+2$ $r_{ij} = r_{(i-1)j} + 2$ else $r_{ij} = r_{(i-1)j} + 4$

- The matrix $D^{D_2}_{d_1(1,1)}$ is equals to $D^{A_2}_{a_1(1,1)}$.
- In matrix $D^{A_2}_{d_1(1,1)}$ the first entry is 4, and other entries of the first row are equal to entries in the second row. We also add one to entries in the first row until $(m-1)^{th}$ row of $D^{A_2}_{a_1(1,1)}$ to obtain the rows from two to m of this matrix.
- The entries of $D^{B_2}_{b_1(1,1)} = [u_{ij}]$ are obtained from $D^{A_2}_{a_1(1,1)}$ the equation $u_{ij} = r_{i(n-j+1)}$
- The matrix $D^{C_2}_{c_1(1,1)}$ is obtained from above equation.
- If we add one by all entries of $D^{B_2}_{b_1(1,1)}$ then we acquire $D^{C_2}_{b_1(1,1)}$.

Table 4. $D^{B_2}_{a_1(1,1)} = [e_{ij}]$.

$i = 1$	$j = 1$	$2 \le j \le n/2$ $(n\vert 2)$ $2 \le j \le (n+1)/2$ $(n\nmid 2)$	$i > 1$	$1 \le j \le n/2$ $(n\vert 2)$ $1 \le j \le (n+1)/2$ $(n\nmid 2)$
	$e_{11}=2$	$e_{1j} = e_{1(j-1)} + 4$		$i \le j$ $e_{ij} = e_{(i-1)j} + 2$ $i > j$ $e_{ij} = e_{(i-1)j} + 4$
$e_{ij} = e_{i(n-j+1)}$ where $[n/2 < j \le n$ & $(n\vert 2)]$ or $[(n+1)/2 < j \le n$ & $(n\nmid 2)]$				

- The matrix $D^{D_2}_{c_1(1,1)}$ is equal to $D^{B_2}_{a_1(1,1)}$.
- Two matrices $D^{C_2}_{a_1(1,1)}$ and $D^{D_2}_{b_1(1,1)}$ achieved by adding 1 to each entry of $D^{B_2}_{a_1(1,1)}$.
- The first and second rows of $D^{A_2}_{b_1(1,1)}$ and $D^{C_2}_{d_1(1,1)}$ are equal and the second until last row of these matrices are computed by adding 2 to the first until $(m-1)^{th}$ row of $D^{B_2}_{a_1(1,1)}$.
- The first and second rows of matrices $D^{A_2}_{c_1(1,1)}$ and $D^{B_2}_{d_1(1,1)}$ are the same and the rows from two to m are equal to the rows from one to $(m-1)$ of $D^{C_2}_{a_1(1,1)}$.
- The matrix $D^{D_1}_{c_1(1,1)} = [z_{ij}]$ obtained from the matrix $D^{B_2}_{a_1(1,1)}$ by relations below;

if $1 \le j \le n/2$ (n is even) or $1 \le j \le (n+1)/2$ (n is odd) then $z_{ij} = e_{ij} - 1$,
and if $n/2 < j \le n$ (n is even) or $(n+1)/2 < j \le n$ (n is odd) then $z_{ij} = e_{ij} + 1$.

- By adding 1 to all entry of $D^{D_1}_{c_1(1,1)} = [d_{ij}]$ we receive to the matrix $D^{D_1}_{b_1(1,1)} = [d_{ij}]$.
- The first and second rows of $D^{A_1}_{c_1(1,1)}$ are equal; and the second until m^{th} row are equal to the first until $(m-1)^{th}$ row of $D^{D_1}_{b_1(1,1)}$.

- The first row of $D^{A_1}_{b_1(1,1)}$ is equal to the first row of $D^{D_1}_{c_1(1,1)}$, and the rows from two to m are obtained by adding 2 to entries of the rows from one to (m−1) of $D^{D_1}_{c_1(1,1)}$.

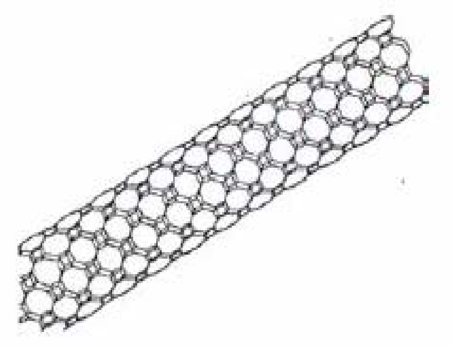

Fig. 1. 3D-Representation of an $TUC_4C_8(S)$ Nanotube.

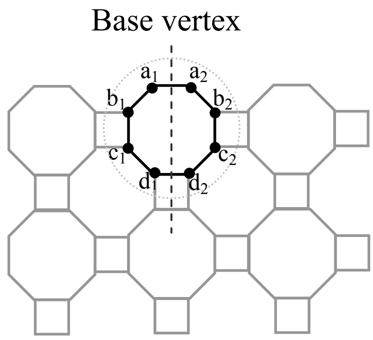

Fig. 2. The basic vertex of T_2

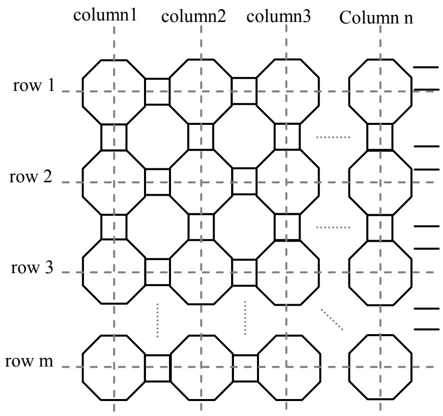

Fig. 3. The 2–Dimensional Fragments of an $TUC_4C_8(S)$ Nanotube.

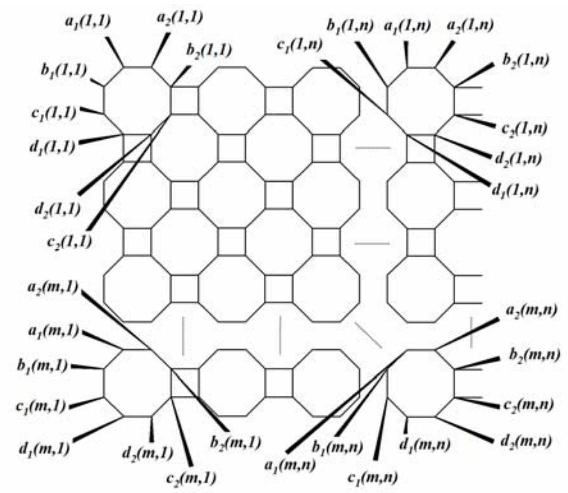

Fig. 4. A Laabeling for T_2

References

[1] H. Wiener, J. Am. Chem. Soc. **69**, 17 (1947).
[2] A. A. Dobrynin, R. Entringer, I. Gutman, Acta Appl. Math., **66**, 211 (2001).
[3] A. A. Dobrynin, I. Gutman, S. Klavžar, P. Zigert, Acta Appl. Math., **72**, 247 (2002).
[4] H .Hosoya, Discr. Appl. Math. **19**, 239 (1988).
[5] B. E. Sagan, Y.-N. Yeh, P. Zhang, Int. J. Quant. Chem. **60**, 959 (1998).
[6] M. V. Diudea M. V., Parv B., Kirby E. C., MATCH Commun. Math. Comput. Chem. **47**, 53 (2003).
[7] M. V. Diudea, Bull. Chem. Soc. Japan **75**, 487 (2002).
[8] M. V. Diudea, MATCH Commun. Math. Comput. Chem. **45**, 109 (2002).
[9] M. V. Diudea, P. E. John, MATCH Commun. Math. Comput. Chem. **44**, 103 (2001).
[10] S. Yousefi, A. R. Ashrafi, J. Math. Chem. **42**, 1031 (2007).
[11] S. Yousefi, A. R. Ashrafi, Curr. Nanosci. **4**, 181 (2008).
[12] A. R. Ashrafi, S. Yousefi, Nanoscale Res. Lett. **2**, 202 (2007).
[13] S. Yousefi, A.R. Ashrafi, MATCH Commun. Math. Comput. Chem. **56**, 169 (2006).
[14] A. R. Ashrafi, S. Yousefi, MATCH Commun. Math. Comput. Chem. **57**, 403 (2007).
[15] S. Yousefi, H. Yousefi-Azari, A. R. Ashrafi, M. H. Khalifeh, J. Sci. Univ. Tehran **33**, 7 (2008).
[16] N. Trinajstic, Chemical Graph Theory, CRC Press, Boca Raton, FL, 1992.

[17] A. Heydari, and B. Taeri, MATCH Commun. Math. Comput. Chem. **57**, 463 (2007).
[18] M. Eliasi, B. Taeri, J. Serb. Chem. Soc. **73**, 311 (2008).
[19] M. Eliasi, B. Taeri, J. Comput. Theor. Nanosci. **4**, 1174 (2007).