A survey on Hosoya polynomial of some nanotubes and nanotori

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ABSTRACT. 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 $G$. In this paper we arrange the main result about the Hosoya polynomial of armchair polyhex, Zig-Zag, TUC$_4$C$_8$(R/S) nanotubes and nanotorus according to Ref.s [23-27].

Keywords: Hosoya polynomial, nanotube, nanotori.

1. INTRODUCTION
Nanotubes and nanotori are an important category of nanostructured materials can be prepared from carbon [1]. These materials are usually represented as molecular graph where the vertices of graph correspond to the atoms and the edges correspond to the chemical bonds. A topological index of a chemical compound is a number related to the molecular graph of compound, describing some of its physic-chemical properties. 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 [2,3].

We now recall some graph theoretical notations that will be used in this paper. Let $G$ be a simple molecular graph without directed and multiple edges without loops and with vertex and edge sets $V(G)$ and $E(G)$, respectively. Suppose $u$ and $v$ are two vertices of $G$. A path between $u$ and $v$ is a sequence of vertices and edges where connect this vertices and the length of path is the number of edges of it. The distance between $u$ and $v$ is a path with minimum cardinality and denoted by $d(u,v)$. The
function \( d(-, -) \) is a metric function on vertex set of \( G \). The diameter of \( G \) is the maximum distance between any pair of vertices, and it is denoted by \( \text{diam}(G) \) [4].

Hosoya polynomial is a counting polynomial introduced by Hosoya in [5] and he proposed the Wiener polynomial for given molecular graph \( G \) for the first time. The roots and coefficients of this polynomial are used for the characterization of topological nature of some chemical compounds. Eventually, it was renamed into “Hosoya polynomial” [6], which name is nowadays most frequently used in the mathematical and mathematico-chemical literature; for further details and references see [7]. The Hosoya polynomial \( W(G, x) \) in the variable \( x \), is defined as the summation of all terms \( d(G, k)x^k \), where \( d(G, k) \) denotes the number of pairs of vertices of the graph \( G \) whose distance is \( k \). Evidently, \( d(G, 0) \) and \( d(G, 1) \) are, respectively, equal to the number of vertices and edges of \( G \), and therefore Hosoya polynomial is a polynomial of degree \( \text{diam}(G) \) [8].

Suppose \( G \) is a molecular graph with vertex set \( V(G) = \{v_1, v_2, ..., v_n\} \). Let \( D = [d_{i,j}]_{n \times n} \) denotes the distance matrix of \( G \), where \( d_{i,j} = d(v_i, v_j) \). Another equivalent way to write the Hosoya polynomial is

\[
W(G, x) = \frac{1}{2} \sum_{j=1}^{n} \sum_{i=1}^{n} x^{d_{i,j}}.
\]

The Hosoya polynomial of \( G \) satisfies in the following conditions:

\[
(W(G, x))' \bigg|_{x=1} = W(G), \quad (xW(G, x))'' \bigg|_{x=1} = 2WW(G) \quad \text{and} \quad (x^2W(G, x))''' \bigg|_{x=1} = 6\text{TSZ}(G),
\]

where \( W(G) \), \( WW(G) \) and \( \text{TSZ}(G) \) are Wiener index [9], hyper-Wiener index [10] and Tratch–Stankevich–Zefirov index [11].

Diudea and his co-authors introduced firstly the problem of computing topological indices of nanomaterials [12-17] and he takes the armchair, zig-zag and \( \text{TUC}_4\text{C}_8(R/S) \) nanotubes into consideration and computed the Wiener index of these nanostructures. Ashrafi and co-authors computed the Wiener index of a polyhex and \( \text{TUC}_4\text{C}_8(R/S) \) nanotori [18-22]. In this paper, we arrange the main results about the computing the Wiener polynomial of armchair polyhex, zig-zag, \( \text{TUC}_4\text{C}_8(R/S) \) nanotubes and nanotori [23-27].

2. Main Results and Discussions

In this section we present the Hosoya polynomial of four classes of carbon nanotubes depicted in Figure 1.
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Figure 1. The Armchair Polyhex, Zig-Zag Polyhex, TUC₄C₈(S) and TUC₄C₈(R) Nanotubes.

2.1 Armchair polyhex carbon nanotube and nanotori

Let TUVC₆[m, n] be the 2–dimensional lattice of Armchair polyhex nanotube, where m is the number of rows and n is the number of zig-zags, and \( V(TUVC₆[m, n]) = \{v(i, j): 1 \leq i \leq m, 1 \leq j \leq n \} \) Figure 2. Define a distance matrix \( D_v(1,1) = [d_{v(1,1)}^{(1,1)}] \) related to vertex \( v(i, j) \) as a base vertex, where \( d_{v(1,1)}^{(1,1)} \) is the distance between the base vertex \( v(1,1) \) and \( v(i, j) \).

Figure 2. The 2–Dimensional Fragment of an Armchair Polyhex Nanotube.
Now, we consider two new matrices as follows:

Matrix A) The first matrix is $A_{\frac{n+1}{2} \times n} = [a_{i,j}]$, where $a_{1,1} = 0$, $a_{2,1} = 1$, $a_{2,2} = 2$, $a_{1,n} = 3$, $a_{2,n} = 2$, and $a_{1,j} = \begin{cases} a_{1,j-1} + 3, & 2 \leq j \leq \frac{n-1}{2} \\ 2j & 2 \leq j \leq \frac{n}{2} \end{cases}$, $2 \leq j \leq n - 1$. Other entries of matrix $A$ are obtained from the first and second rows by equations $a_{i,j} = a_{1,j}$ where $2 \leq i$, and $a_{i,j} = a_{2,j}$, otherwise.

Matrix B) The second matrix is $B_{\frac{n+1}{2} \times n} = [b_{i,j}]$, where $b_{\frac{n+1}{2}+1,j} = \begin{cases} \frac{n}{2} + j - 1, & j \leq \frac{n}{2} + 1 \\ 3n - j + 1, & j > \frac{n}{2} + 1 \end{cases}$ and $b_{i,j} = b_{i+1,j} - 1$ ($1 \leq i \leq \frac{n}{2}$).

Then the entries of distance matrix of $TUVC_6[m,n]$ related to the base vertex $v(1,1)$ is equals to $d_{i,j}^{v(1,1)} = \begin{cases} \max\{a_{i,j},b_{i,j}\}, & j \leq \frac{n}{2} + 1 \\ d_{i-1,j}, & j > \frac{n}{2} + 1 \end{cases}$. Suppose $\Delta_1, \Delta_2, ..., \Delta_m$ are rows of $D_{v(1,1)}$ and Define permutation functions $\alpha_i$ and $\beta_j$ as follow:

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

$$\beta_j = \begin{pmatrix} 1 & 2 & \hdots & j-1 & j & \hdots & n \\ n-j+2 & n-j+3 & \hdots & n & 1 & \hdots & n-j+1 \end{pmatrix}; \text{ } j \text{ is odd},$$

$$\beta_j = \begin{pmatrix} 1 & 2 & \hdots & j & j+1 & j+2 & \hdots & n \\ j & j-1 & \hdots & 1 & n & n-1 & \hdots & j+1 \end{pmatrix}; \text{ } j \text{ is even}.$$
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In this equation, we enumerate the entries of distance matrix $D_1 = D(TUVC[m,n])$. The entries of $\Delta_1$ are appear $mn$ times in $D_1$ and the entries of $\Delta_i$ are appear $2n(m - i + 1)$ times where $2 \leq i \leq m$. Therefore the Hosoya polynomial of $T_1 = TUVC[m,n]$ is equals to:

$$W(T_1, x) = \frac{1}{2} n \left[ m \sum_{j=1}^{n} x^{d^1_{i,j}} + \sum_{i=2}^{m} 2(m - i + 1) \left( \sum_{j=1}^{n} x^{d^1_{i,j}} \right) \right].$$

Now, consider the distance matrix $D_2$ of an armchair polyhex carbon nanotube $S_1$. By apply a similar algorithm as above, we obtain $D_{v(i,j)} = \beta_{j} a_{m} D_{v(1,1)}$. By this equation the Wiener polynomial of $S_1$ is as follows:

$$W(S_1, x) = \frac{mn}{2} \left( \sum_{j=1}^{n} x^{d^1_{i,j}} + 2 \left( \sum_{i=2}^{m} \sum_{j=1}^{n} x^{d^1_{i,j}} \right) + \sum_{j=1}^{m} x^{d_{m}^1_{i,j}} \right).$$

2.2 Zig-zag polyhex carbon nanotube

Let $T_2 = TUVC_{6}[m,n]$ be the zig–zag polyhex carbon nanotube, where $m$ is the number of rows and $n$ is the number of zig-zags and it is an even integer, Figure 3.

Choose two base vertices $v(1,1)$ and $u(1,1)$ from the 2–dimensional lattice of $T_2$. Let $D_{u(1,1)} = [d_{u,j}^{(1,1)}]$ and $D_{v(1,1)} = [d_{i,j}^{(1,1)}]$ are distance matrices between vertex $u(1,1)$ and vertex $v(1,1)$ and all vertices of $T_2$, respectively. Define three matrices as follows:

$$A_{u(1,1)}^{m,n} = [a_{i,j}];$$

$$a_{1,1} = 0, a_{1,2} = 1, a_{i,1} = \begin{cases} a_{i-1,1} + 1, 2| i \\ a_{i,2} + 1, 2 \nmid i \end{cases}$$

$$a_{i,2} = \begin{cases} a_{i-1,2} + 1, 2| i \\ a_{i,2} + 1, 2 \nmid i \end{cases}$$

and $a_{i,j} = \begin{cases} a_{i,1}, 2 \mid j \\ a_{i,2}, 2 \nmid j \end{cases}.$
Figure 3. The 2–Dimensional Fragment of an Zig–Zag Polyhex Carbon Nanotube.

\[ A^{\nu(1,1)}_{m \times (n/2+1)} = [c_{i,j}]: \]

\[ c_{1,1} = 0, \ c_{1,2} = 1, \ c_{i,1} = \begin{cases} c_{i,1} + 1, & 2 | i \\ c_{i-1,1} + 1, 2 \nmid i & c_{i,2} = \begin{cases} c_{i-1,2} + 1, 2 | i \\ c_{i,1} + 1, 2 \nmid i \end{cases} \end{cases} \quad \text{and} \quad c_{i,j} = \begin{cases} c_{i,1}, & 2 \nmid j \\ c_{i,2}, & 2 | j \end{cases} \]

\[ B_{m \times (n/2+1)} = [b_{i,j}]: b_{i,1} = i - 1 \ \text{where} \ 1 \leq i \leq m \ \text{and} \ b_{i,j} = b_{i,j-1} + 1 \ \text{for} \ \text{other} \ \text{entries}. \]

From these matrices, one can easily compute matrices \( D_{u(1,1)} \) and \( D_{v(1,1)} \) as follows:

\[ d_{ij}^{u(1,1)} = \begin{cases} \max(a_{ij}, b_{ij}) & 1 \leq j \leq n/2 + 1 \\ c_{i(j-n/2)}^{u(1,1)} & j > n/2 + 1 \end{cases} \quad d_{ij}^{v(1,1)} = \begin{cases} \max(a_{ij}, c_{ij}) & 1 \leq j \leq n/2 + 1 \\ d_{i(j-n/2)}^{v(1,1)} & j > n/2 + 1 \end{cases} \]

Now, set \( D_{u(1,1)} = [\Delta_{i}^{u(1,1)}]_{1 \leq i \leq m} \) and \( D_{v(1,1)} = [\Delta_{i}^{v(1,1)}]_{1 \leq i \leq m} \), such that \( \Delta_{i} \) denotes the \( i \)th row of the matrix. We also assume that the first row of \( D_{u(1,1)} \) and \( D_{v(1,1)} \) are as follows:

\[ [d_{u(1,1)}^{u(1,1)}, d_{u(1,2)}^{u(1,1)}, \ldots, d_{u(1,n/2)}^{u(1,1)}, d_{u(1,n/2)}^{u(1,1)}, d_{v(1,1)}^{u(1,1)}]. \]
Therefore the Hosoya polynomial of $T_2$ is as follows:

$$W(T, x) = W_u(T, x) + W_v(T, x)$$
2.3 TUC$_4$C$_8$(S) carbon nanotube and nanotori

Suppose $T_3$ is 2–dimensional lattice of TUC$_4$C$_8$(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 4. Consider partition $P = \{A_1, A_2, B_1, B_2, C_1, C_2, D_1, D_2\}$ of $V(T_3)$ in which if $X_j \in P$ then $X_j = \{x_k(i,t): 1 \leq i \leq m, 1 \leq t \leq n, k = j\}$. The matrix $D^{X_j}_{x_k(1,1)}$ is a matrix in which its entries are the distance from $x_k(1,1)$ to all of vertices in $X_j$. To compute distance matrix of $T_3$, we must find all of these matrices. The first row of $D(T_3)$ is the all entries of eight matrices of vertex $a_1(1,1)$, and other rows are obtained similarly. By using the symmetry of $T_3$, we don’t need to investigate the vertices with subscript 2. Hence the computation of sixty four matrices presented above, decreases to thirty two matrices.

Let $D^{X_j}_{x_k(1,1)} = [(X^{x_k}_j)_{i}]_{1 \leq i \leq m}$ where $(X^{x_k}_j)_{i}$ is $i$th row of the matrix and $k \in \{1,2\}$. We can obtain other matrices for the $t$th row ($2 \leq t \leq m$) and first column of $T_3$. Now we enumerate the entries of distance matrix $D(T_3)$. For this, define $\alpha_i$ ($1 \leq i \leq m$), by

Figure 4. The 2–Dimensional Fragment of an TUC$_4$C$_8$(S) Carbon Nanotube.
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\[ \alpha_i = \begin{pmatrix} 1 & 2 & \ldots & i & i + 1 & \ldots & m \\ i & i - 1 & \ldots & 1 & 2 & \ldots & m - i + 1 \end{pmatrix} \]

Then we can see that the times of repeating \( s \)-th row matrix \( D_{x_j(1,1)} \) is the number of columns in \( T_3 \) multiplied by the number of members of the set \( \{ \alpha(j+s-1), \alpha(j-s+1) : j, j+s-1, j-s+1 \leq m \} \). Therefore, for this matrix we obtain the following polynomial:

\[
W_{x_j(1,1)}^{x_j}(T_3, x) = \frac{1}{2} \times 2^n \left[ m \sum_{j=1}^{n} x^{d_{i,j}} \right] + \sum_{i=2}^{m} 2(m-i+1) \left( \sum_{j=1}^{n} x^{d_{i,j}} \right) \]

So the Wiener polynomial of \( T_3 \) is \( W(T_3, x) = \sum_{x_j, x_k} W_{x_j(1,1)}^{x_j}(T_3, x) \).

Now consider the molecular graph of a \( S_3 = TUC_4C_8(S) [m,n] \) nanotorus, where \( m \) is the number of rows and \( n \) is the number of columns. As similar way, 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 5.

![Figure 4](image)

Figure 4. The 2–Dimensional Fragment of an TUC4C8(S) Carbon Nanotori.
Also, partition $V(S_3)$ into eight parts $P = \{A_1, A_2, B_1, B_2, C_1, C_2, D_1, D_2\}$ where $X_j \in P$ and $X_j = \{x_k(i,t) \mid 1 \leq i \leq m, 1 \leq t \leq n, k = j\}$. To compute $D(S_3)$, it is enough to calculate matrices $D_{x_k(1,1)}^{X_j}$. By a similar argument as above, we obtain the following polynomial as

$$W_{x_k(1,1)}^{X_j}(S_3, x) = \frac{1}{2} nm \sum_{i,j} x^{d_{i,j}} \text{ for matrix } D_{x_k(1,1)}^{X_j}.$$ 

Therefore the Hosoya polynomial of $S_3$ is equals to $W(S_3, x) = 2 \times \sum_{X_j, X_1} W_{x_1(1,1)}^{X_j}(S_3, x)$.

### 2.4 TUC₄C₈(R) nanotube and nanotori

Let $T_4$ be 2–dimensional lattice of TUC₄C₈(R)[m,n], where $m$ is the number of rows and $n$ is the number of columns of it. Similar as last section, choose four base vertices $x(1,1), x \in \{a, b, c, d\}$ from the molecular graph of $T_4$, Figures 5.

**Figure 5.** The 2–Dimensional Fragment of TUC₄C₈(R) Carbon Nanotube.

Partition the vertex set of $T_4$ into four sets $A, B, C$, and $D$ such that all vertices with label $a$ are in the set $A$, and so on. Define matrix $D_{a(1,1)}^{d(i,j)}$ as the matrix for the base
vertex $a(1,1)$ in which the entries of this matrix are distances between $a(1,1)$ and $a(i,j)$ in $A$. For computing $D(T_4)$, we first define the following 16 matrices:

$$
\begin{align*}
D_{a(1,1)}^A, D_{a(1,1)}^B, D_{a(1,1)}^C, D_{a(1,1)}^D, D_{a(1,1)}^A, D_{b(1,1)}^B, D_{b(1,1)}^C, D_{b(1,1)}^D, \\
D_{c(1,1)}^A, D_{c(1,1)}^B, D_{c(1,1)}^C, D_{c(1,1)}^D, D_{a(1,1)}^A, D_{a(1,1)}^B, D_{a(1,1)}^C, D_{a(1,1)}^D.
\end{align*}
$$

By using the symmetry of $T_4$, it is enough to compute eight of these matrices. Remark that four matrices $D_{a(1,1)}^{a(i,j)}, D_{b(1,1)}^{b(i,j)}, D_{c(1,1)}^{c(i,j)}$ and $D_{d(1,1)}^{d(i,j)}$ are equal. Consider the permutation $\mu = \begin{pmatrix} 1 & 2 & 3 & \ldots & n-1 & n \\ 1 & n & n-1 & \ldots & 3 & 2 \end{pmatrix}$. One can easily see that the matrices $D_{b(1,1)}^{b(i,j)}$ and $D_{c(1,1)}^{c(i,j)}$ are obtained from $D_{a(1,1)}^{d(i,j)}$ and $D_{a(1,1)}^{d(i,j)}$. By symmetry of $T_4$, it is possible to compute the matrix evaluated at the base vertex $d$ from the same matrix for the vertex $b$. On the other hand, the matrices $D_{b(1,1)}^{d(i,j)}, D_{d(1,1)}^{d(i,j)}$ and $D_{d(1,1)}^{d(i,j)}$ is computed from $D_{a(1,1)}^{d(i,j)}, D_{b(1,1)}^{d(i,j)}$ and $D_{b(1,1)}^{d(i,j)}$ by trace of $\mu$.

We now count the repeated entries of these matrices to find the following equation:

$$
W^{a(i,j)}_{a(1,1)}(T_4, x) = \frac{1}{2n} \left[ m \left( \sum_{j=1}^{n} x^{d_{1,j}} \right) + \sum_{i=2}^{m} 2(m - i + 1) \left( \sum_{j=1}^{n} x^{d_{i,j}} \right) \right],
$$

where $D_{a(1,1)}^{a(i,j)} = [d_{i,j}]$.

Other polynomials are similar and so the Hosoya polynomial of this nanotube is computed as follows:
\[ W(TUC_4C_8(R), x) = 4W^{a(i,j)}_{a(1,1)}(TUC_4C_8(R), x) + 2W^{d(i,j)}_{a(1,1)}(TUC_4C_8(R), x) + W^{c(i,j)}_{a(1,1)}(TUC_4C_8(R), x) + 2W^{d(i,j)}_{c(1,1)}(TUC_4C_8(R), x) + 2W^{d(i,j)}_{b(1,1)}(TUC_4C_8(R), x) + 2W^{d(i,j)}_{b(1,1)}(TUC_4C_8(R), x). \]

Now consider the molecular graph of a \( S_4 = TUC_4C_8(R) \) nanotorus. For this molecular graph, choose four base vertices \( a(i,j), b(i,j), c(i,j) \) and \( d(i,j) \), Figure 6.

**Figure 6.** The 2–Dimensional Fragment of TUC_4C_8(R) Carbon Nanotori.

By apply similar argument and consider partition \( A, B, C \) and \( D \) for vertices, we found the polynomial \( W^A_6(T_4, x) = \frac{1}{2} nm \sum_{j=1}^{n} \sum_{i=1}^{m} x^{d_{ij}} \), where \( D^A_{d(1,1)} = [d_{ij}] \). Other polynomials are similar and so the Hosoya polynomial of this nanotorus is computed as follows:

\[
H(T, q) = 4H^A_6(T, q) + 2H^D_6(T, q) + H^C_6(T, q) + H^A_6(T, q) + 2H^D_6(T, q) + 2H^D_6(T, q).
\]

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