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Hosoya polynomial of zigzag polyhex nanotorus

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Abstract: The Hosoya polynomial of a molecular graph G is defined as $H(G,\lambda)=\sum_{\{u,v\}\subseteq V(G)}\lambda^{d(u,v)}$, where $d(u,v)$ is the distance between vertices u and v. The first derivative of $H(G,\lambda)$ at $\lambda = 1$ is equal to the Wiener index of G, defined as $W(G)=\sum_{\{u,v\}\subseteq V(G)}d(u,v)$. The second derivative of $\frac{1}{2}\lambda H(G,\lambda)$ at $\lambda=1$ is equal to the hyper-Wiener index, defined as $WW(G)=\frac{1}{2}W(G)+\frac{1}{2}\sum_{\{u,v\}\subseteq V(G)}d(u,v)^2$. Xu *et al.*[1] computed the Hosoya polynomial of zigzag open-ended nanotubes. Also Xu and Zhang[2] computed the Hosoya polynomial of armchair open-ended nanotubes. In this paper, a new method was implemented to find the Hosoya polynomial of $G = HC_6[p,q]$, the zigzag polyhex nanotori and to calculate the Wiener and hyper Wiener indices of G using $H(G,\lambda)$.

Keywords: Wiener index; hyper-Wiener index; Hosoya polynomial; nanotubes.

INTRODUCTION

A topological index is a real number related to a structural graph of a molecule. It does not depend on the labeling or pictorial representation of graph. Among topological indices, the Wiener index[3] is certainly the most important one. This index was introduced by the chemist Harold Wiener, about 60 years ago to demonstrate correlations between physico-chemical properties of organic compounds and the topological structure of their molecular graphs. Wiener defined his index as the sum of the distances between two carbon atoms in the molecules, in terms of carbon–carbon bonds. The historical details and further bibliography on the chemical applications of the Wiener index are reviewed in the literature.[4,5]

The topological distance between a pair of vertices u and v of a molecular graph G, denoted by $d(u,v)$, is the number of edges on the shortest path joining u and v. Thus, the Wiener index of G is half the sum of distances between all vertices of the graph G:

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

where $V(G)$ is the set of vertices of G.

Another topological index is the hyper-Wiener index that was defined by Klein *et al.*[6] and others[7–12] applied it to cyclic structures as:

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

Haruo Hosoya[13] introduced a distance-based polynomial, which he called the Wiener polynomial, related to each connected graph G as:

$$H(G,\lambda)=\sum_{k\geq 0} d(G,k)\lambda^k$$

where $d(G,k)$ is the number of pair vertices of G that are at distance k of each other. However, today it is called the Hosoya polynomial.[14–15] It is easy to see that it is equal to:

$$H(G,\lambda)=\sum_{\{u,v\}\subseteq V(G)} \lambda^{d(u,v)}$$

In 1991, Iijima[16] discovered carbon nanotubes as multi-walled structures. Carbon nanotubes show remarkable mechanical properties. Experimental studies have shown that they belong to the stiffest and most elastic materials known. These mechanical characteristics clearly predestinate nanotubes for advanced composites. Diudea was the first chemist who considered the problem of computing topological indices of nanostructures.[1,2,17–24] Recently computing topological indices of nanostructures has been the subject of many papers. The reader is encouraged to consult papers[25–31] on computing topological indices of some nanotubes.

RESULTS AND DISCUSSION

Xu *et al.*[1] computed the Hosoya polynomials of zigzag open-ended nanotubes. Also Xu and Zhang[2] computed the Hosoya polynomial of polynomials of armchair open-ended nanotubes. In this paper, a new method was implemented to find the Hosoya polynomial of zigzag polyhex nanotorus. Throughout this paper, $G = HC_6[p,q]$ (see Fig. 1) denotes an arbitrary zigzag polyhex nanotorus in terms of the circumference p and the length q.

It should be noticed that p and q must be even. Also, a coordinate label for the vertices of $G = HC_6[p,q]$, as shown in Fig. 2, was chosen. The distances from x_{01} to all vertices are given in Fig. 3. Note that the graph is bipartite, or equivalently, the vertices can be colored with white and black, so that adjacent vertices have a different color. Since the graph is symmetric with respect to the line joining $x_{0,\frac{p}{2}+1}$ to $x_{1,\frac{p}{2}+1}$, one half of the numbers are shown in Fig. 3.

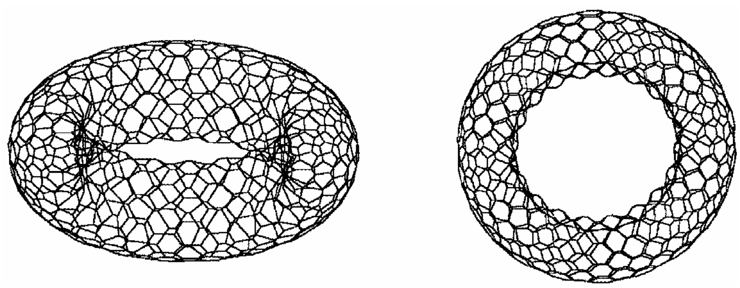

Fig. 1. $HC_6[20,40]$: Side view; top view.

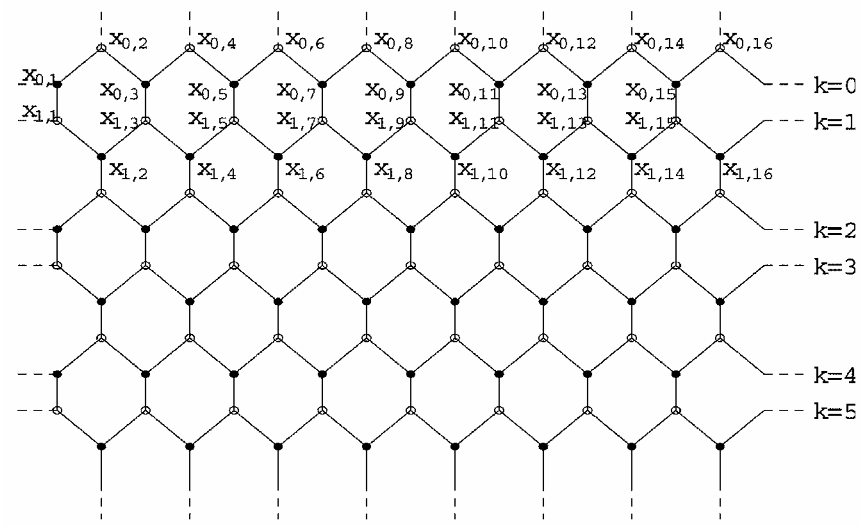

Fig. 2. A zigzag polyhex nanotorus lattice with $p = 16$ and $q = 6$.

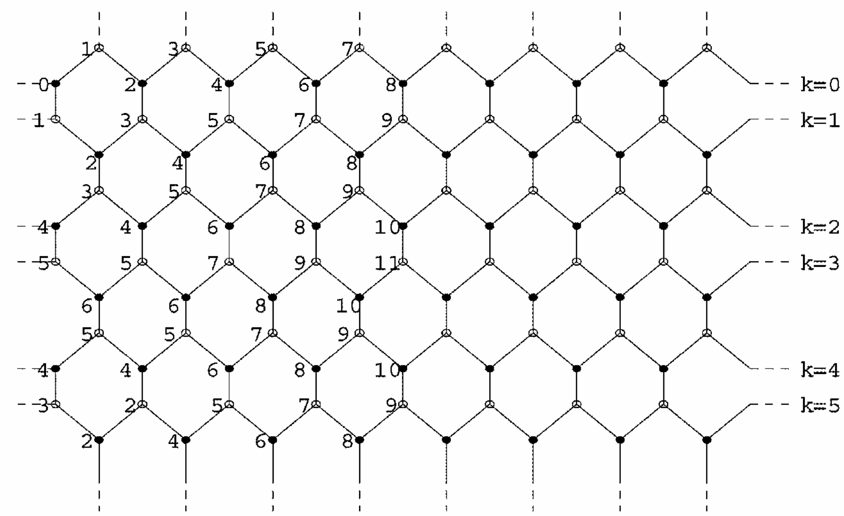

Fig. 3. Distances from x_{01} to each vertex of $HC_6[6,16]$.

CALCULATION PROCEDURE

For a vertex $u \in V(G)$,

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

is defined and the work is commenced with the following key result.

Result 1. Let $u \in V(G)$ be a white vertex and the summation of $\lambda^{\alpha(u,x)}$, where x varies on the vertices of level k, is denoted by $w_k(\lambda)$. Then if $0 \le k < p/2$, one obtains:

$$\begin{aligned} w_k(\lambda) &= \sum_{x \in \text{level}\, k} \lambda^{d(x_{02},x)} \\ &= \sum_{x \in \text{level}\, k} \lambda^{d(x_{04},x)} \\ &\vdots \\ &= \frac{1}{\lambda-1}\left(\lambda^{k+\frac{p}{2}} - \lambda^{2k+1} + \lambda^{k+\frac{p}{2}+1} - k\lambda^{2k} - \lambda^{2k} + k\lambda^{2k+2}\right) \end{aligned}$$

and if $k \ge p/2$ then one has:

$$\begin{aligned} w_k(\lambda) &= \sum_{x \in \text{level}\, k} \lambda^{d(x_{02},x)} \\ &= \sum_{x \in \text{level}\, k} \lambda^{d(x_{04},x)} \\ &\vdots \\ &= \frac{p}{2}\lambda^{2k+1} + \frac{p}{2}\lambda^{2k} \end{aligned}$$

Similarly, suppose that $u \in V(G)$ is a black vertex and the summation of $\lambda^{\alpha(u,x)}$, where x varies on the vertices of level k, is denoted by $b_k(\lambda)$. Then if $0 \le k < p/2$, one has:

$$\begin{aligned} b_k(\lambda) &= \sum_{x \in \text{level}\, k} \lambda^{d(x_{01},x)} \\ &= \sum_{x \in \text{level}\, k} \lambda^{d(x_{03},x)} \\ &= \frac{1}{\lambda-1}\left(\lambda^{k+\frac{p}{2}} - \lambda^{2k+1} + \lambda^{k+\frac{p}{2}+1} + k\lambda^{2k+1} - \lambda^{2k} - k\lambda^{2k-1}\right) \end{aligned}$$

and if $k \ge p/2$, then one has:

$$\begin{aligned} b_k(\lambda) &= \sum_{x \in \text{level}\, k} \lambda^{d(x_{01},x)} \\ &= \sum_{x \in \text{level}\, k} \lambda^{d(x_{03},x)} \\ &= \frac{p}{2}\lambda^{2k-1} + \frac{p}{2}\lambda^{2k} \end{aligned}$$

Proof. $b_k(\lambda)$ is computed. It is suffices to consider x_{01}. For other black vertices, the argument is similar. Firstly, note that the lattice is symmetric with respect to the line joining x_{01} to x_{11}. Three cases can be distinguished:

Case 1. $p/2 \le k$ and k is even. In this case, for all $1 \le j \le p/2 + 1$, one has

$$d(x_{01}, x_{kj}) = \begin{cases} 2k-1 & \text{if } j \text{ is even} \\ 2k & \text{if } j \text{ is odd} \end{cases}$$

Now by considering these vertices and their symmetric vertices, one obtains $p/2$ vertices having a distance $2k-1$ from x_{01}, and $p/2$ vertices having a distance $2k$ from x_{01}. Hence,

$$b_k(\lambda) = \frac{p}{2}\lambda^{2k-1} + \frac{p}{2}\lambda^{2k}$$

Case 2. $p/2 \le k$ and k is odd. In this case for all $1 \le j \le p/2+1$, one has:

$$d(x_{01}, x_{kj}) = \begin{cases} 2k & \text{if } j \text{ is even} \\ 2k-1 & \text{if } j \text{ is odd} \end{cases}$$

Now by considering these vertices and their symmetric vertices, one obtains $p/2$ vertices having distance $2k-1$ from x_{01}, and $p/2$ vertices having a distance $2k$ from x_{01}. Hence,

$$b_k(\lambda) = \frac{p}{2}\lambda^{2k-1} + \frac{p}{2}\lambda^{2k} .$$

Case 3. $p/2 < k$. For all j's, such that $p + 1 \le j$ and $k + 1 < j$, one has:

$$d(x_{01}, x_{kj}) = k + j - 1$$

Thus, the summation of the distances between x_{01} and x_{kj} (for all j's, such that $p + 1 \le j$ and $k + 1 < j$) and their symmetric vertices is:

$$S_1 = 2\sum_{j=k+2}^{\frac{p}{2}} \lambda^{k+j-1} + \lambda^{k+\frac{p}{2}+1-1} = \frac{1}{\lambda-1}(\lambda^{k+\frac{p}{2}} - 2\lambda^{2k+1} + \lambda^{k+\frac{p}{2}+1})$$

Also if $1 \le j \le k + 1$, then

$$d(x_{01}, x_{kj}) = \begin{cases} 2k & \text{if } k-j \text{ is odd} \\ 2k-1 & \text{if } k-j \text{ is even} \end{cases}$$

Therefore, the summation of the distances between x_{01} and x_{kj} (for all j such that$1 \le j \le k + 1$) and their symmetric vertices is:

$$S_2 = (k+1)\lambda^{2k} + k\lambda^{2k-1}$$

Hence,

$$b_k(\lambda) = S_1 + S_2 = \frac{1}{\lambda-1}(\lambda^{k+\frac{p}{2}} - \lambda^{2k+1} + \lambda^{k+\frac{p}{2}+1} + k\lambda^{2k+1} - \lambda^{2k} - k\lambda^{2k-1})$$

The proof for $w_k(\lambda)$is similar.

Result 2. For one white or black vertex x_{0j} of level 0, one has:

$$w_{\frac{q}{2}}(\lambda) = b_k(\lambda) := \sum_{x \in \text{level}\frac{q}{2}} \lambda^{d(x_{0j},x)} =$$

$$= \begin{cases} \frac{1}{\lambda-1}(\lambda^{\frac{q}{2}+\frac{p}{2}} - \lambda^{2(\frac{q}{2})+1} + \lambda^{\frac{q}{2}+\frac{p}{2}+1} + \frac{q}{2}\lambda^{2(\frac{q}{2})+1} - \lambda^{2(\frac{q}{2})} - (\frac{q}{2})\lambda^{2(\frac{q}{2})-1}) & \text{if } \frac{q}{2} < \frac{p}{2} \\ \frac{p}{2}\lambda^{2(\frac{q}{2})-1} + \frac{p}{2}\lambda^{2(\frac{q}{2})} & \text{if } \frac{q}{2} \ge \frac{p}{2} \end{cases}$$

Proof. Since G is symmetric with respect to the line joining x_{01} to x_{11}, it is sufficient to prove the assertion for x_{01} and x_{02}. For x_{01}, the proof is exactly the proof of Result 1. Considering tori that can be built up from two halves collapsing at level 0, the top part x_{02} is a black vertex, hence by the proof of Result 1, one can calculate $b_{\frac{q}{2}}(\lambda)$.

Result 3. For each $u \in V(G)$, one has:

$$D(\lambda) := d(u,\lambda) = b_0(\lambda) + b_1(\lambda) + \cdots + b_{\frac{q}{2}}(\lambda) + w_1(\lambda) + \cdots + w_{\frac{q}{2}-1}(\lambda)$$

Proof. Firstly, note that the lattice is symmetric (with respect to the level k). Hence, it suffices to consider x_{01} and x_{02}. For other black (white) vertices, the argument is similar. Now, beginning with x_{01}, let $B_1 = \{k \mid 0 \le k \le \frac{q}{2}\}$ and $B_2 = \{k \mid \frac{q}{2} < k \le q-1\}$. Then one has:

$$d(x_{01},\lambda) = \sum_{v \in V(G)} \lambda^{d(x_{01},v)} = \sum_{v \in B_1} \lambda^{d(x_{01},v)} + \sum_{v \in B_2} \lambda^{d(x_{01},v)}$$

However,

$$\sum_{v \in B_1} \lambda^{d(x_{01},v)} = \sum_{v \in level 0_1} \lambda^{d(x_{01},v)} + \sum_{v \in level 1_1} \lambda^{d(x_{01},v)} + \cdots + \sum_{v \in level_1 \frac{q}{2}-1} \lambda^{d(x_{01},v)} = b_0(\lambda) + b_1(\lambda) + \cdots + b_{\frac{q}{2}}(\lambda)$$

For computing the last sum, tori that can be built up from two halves collapsing at level 0 are considered. The top part is formed of the lines of B_2 such that x_{01} are a black vertex. Hence, by changing the index and using the proof of Lemma 1, one obtains:

$$\sum_{v \in B_2} \lambda^{d(x_{01},v)} = \sum_{v \in \mathrm{level} q-1_1} \lambda^{d(x_{01},v)} + \sum_{v \in \mathrm{level} q-2_1} \lambda^{d(x_{01},v)} + \cdots + \sum_{v \in \mathrm{level}_1 \frac{q}{2}+1} \lambda^{d(x_{01},v)} = w_1(\lambda) + \cdots + w_{\frac{q}{2}-1}(\lambda)$$

which completes the proof.

Theorem. The Hosoya polynomial, $H(G,\lambda)$, of $G = HC_6[p,q]$, nanotorus is given by:

$$\begin{cases} H_1(G,\lambda) & \text{if } q \le p \\ H_2(G,\lambda) & \text{if } q > p \end{cases}$$

where

$$H_1(G,\lambda) = \frac{pq}{4\lambda(\lambda-1)^2}(-2\lambda^{q+2} + 2\lambda^{\frac{p}{2}+\frac{q}{2}+2} - 2\lambda^{\frac{p}{2+2}} + 4\lambda^2 + q\lambda^{q+2} + \\ +4\lambda^{\frac{p}{2}+\frac{q}{2}+1} - 4\lambda^{\frac{p}{2}+1} - 2\lambda^{q+1} - 2\lambda - 2\lambda^{\frac{p}{2}} - 2\lambda^q + 4 - q\lambda^q + 2\lambda^{\frac{p}{2}+\frac{q}{2}})$$

and

$$H_2(G,\lambda) = \frac{pq}{4\lambda(\lambda-1)^2}(-2\lambda^{\frac{p}{2}+3} + p\lambda^{q+3} + 4\lambda^3 - 4\lambda^{p+2} - p\lambda^{p+2} - \\ -4\lambda^{\frac{p}{2}++2} - 2\lambda^2 + p\lambda^{p+1} + 4\lambda^{p+2} + 4\lambda^{p+1} + 4\lambda - 2\lambda^{\frac{p}{2}+1} - 4\lambda^{p+1} - p\lambda^{q+1})$$

Proof. One has:

$$H(G,\lambda) = \frac{1}{2}\sum_{u \in V(G)}\sum_{v \in V(G)} \lambda^{d(u,v)} + \frac{1}{2}\sum_{u \in V(G)} \lambda^{d(u,u)} = \frac{1}{2}\sum_{v \in V(G)} d(v,\lambda) + \frac{1}{2}|V(G)| = \frac{1}{2}\sum_{v \in V(G)} D(\lambda) + \frac{1}{2}pq = \\ = \frac{pq}{2}D(\lambda) + \frac{1}{2}pq$$

First suppose that $q \le p-2$. In this case, $q < p$, hence by Result 3 and Result 1, one has:

$$D(\lambda) = b_o(\lambda) + b_1(\lambda) + \cdots + b_{\frac{q}{2}}(\lambda) + w_1(\lambda) + \cdots + w_{\frac{q}{2}-1}(\lambda)$$

$$= \sum_{k=0}^{\frac{q}{2}} \frac{1}{\lambda-1}(\lambda^{k+\frac{p}{2}} - \lambda^{2k+1} + \lambda^{k+\frac{p}{2}+1} + k\lambda^{2k+1} - \lambda^{2k} - k\lambda^{2k-1})$$

$$\sum_{k=1}^{\frac{q}{2}-1} \frac{1}{\lambda-1}(\lambda^{k+\frac{p}{2}} - \lambda^{2k+1} + \lambda^{k+\frac{p}{2}+1} - k\lambda^{2k} - \lambda^{2k} + k\lambda^{2k+2}) =$$

$$= \frac{1}{2\lambda(\lambda-1)(\lambda^2-1)}(2\lambda + 4\lambda^2 + q\lambda^{q+3} - 4\lambda^{q+2} + 2\lambda^4 + 4\lambda^3 -$$

$$-2\lambda^{q+4} - 4\lambda^{q+3} + 2\lambda^{\frac{p}{2}+4+\frac{q}{2}} + 6\lambda^{\frac{p}{2}+3+\frac{q}{2}} + 6\lambda^{\frac{p}{2}+2+\frac{q}{2}} - 6\lambda^{\frac{p}{2}+3} -$$

$$-6\lambda^{\frac{p}{2}+2} - 2\lambda^{\frac{p}{2}+1} - q\lambda^{2+q} + q\lambda^{q+4} - q\lambda^{1+q} - 2\lambda^{q+1} + 2\lambda^{\frac{p}{2}+3+\frac{q}{2}} - 2\lambda^{\frac{p}{2}+4})$$

Hence, in this case $H(G,\lambda) = H_1(G,\lambda)$.

Now suppose that $p \le q-2$. In this case, $p/2-1 \le q/2-1$, hence by Result 3 and Result 1, one has:

$$D(\lambda) = b_0(\lambda) + b_1(\lambda) + \cdots + b_{\frac{q}{2}}(\lambda) + w_1(\lambda) + \cdots + w_{\frac{q}{2}-1}(\lambda) =$$

$$= b_0(\lambda) + b_1(\lambda) + \cdots + b_{\frac{p}{2}-1}(\lambda) + b_{\frac{p}{2}}(\lambda) + \cdots + b_{\frac{q}{2}}(\lambda) +$$

$$+ w_1(\lambda) + \cdots + w_{\frac{p}{2}-1}(\lambda) + w_{\frac{p}{2}}(\lambda) + \cdots + w_{\frac{q}{2}-1}(\lambda) =$$

$$= \sum_{k=0}^{\frac{p}{2}-1} \frac{1}{\lambda-1}(\lambda^{k+\frac{p}{2}} - \lambda^{2k+1} + \lambda^{k+\frac{p}{2}+1} + k\lambda^{2k+1} - \lambda^{2k} - k\lambda^{2k-1}) +$$

$$+ \sum_{k=\frac{p}{2}}^{\frac{q}{2}} (\tfrac{p}{2}\lambda^{2k-1} + \tfrac{p}{2}\lambda^{2k}) + \sum_{k=1}^{\frac{p}{2}-1} \frac{1}{\lambda-1}(\lambda^{k+\frac{p}{2}} - \lambda^{2k+1} + \lambda^{k+\frac{p}{2}+1} - k\lambda^{2k} - \lambda^{2k} + k\lambda^{2k+2}) +$$

$$+ \sum_{k=\frac{p}{2}}^{\frac{q}{2}-1} (\tfrac{p}{2}\lambda^{2k+1} + \tfrac{p}{2}\lambda^{2k})$$

After calculation of these summations, one obtains:

$$H(G,\lambda) = H_2(G,\lambda)$$

Finally, if $p = q$, then by Result 3 and Result 1, for each $u \in V(G)$, one has:

$$D(\lambda) = b_0(\lambda) + b_1(\lambda) + \cdots + b_{\frac{q}{2}}(\lambda) + w_1(\lambda) + \cdots + w_{\frac{q}{2}-1}(\lambda) =$$

$$= b_0(\lambda) + b_1(\lambda) + \cdots + b_{\frac{p}{2}-1}(\lambda) + w_{\frac{p}{2}}(\lambda) + w_1(\lambda) + \cdots + w_{\frac{p}{2}-1}(\lambda) =$$

$$= \sum_{k=0}^{\frac{p}{2}-1qp} \frac{1}{\lambda-1}(\lambda^{k+\frac{p}{2}} - \lambda^{2k+1} + \lambda^{k+\frac{p}{2}+1} + k\lambda^{2k+1} - \lambda^{2k} - k\lambda^{2k-1}) + (\tfrac{p}{2}\lambda^{2(\frac{p}{2})-1} + \tfrac{p}{2}\lambda^{2(\frac{p}{2})})$$

$$\sum_{k=1}^{\frac{p}{2}-1} \frac{1}{\lambda-1}(\lambda^{k+\frac{p}{2}} - \lambda^{2k+1} + \lambda^{k+\frac{p}{2}+1} - k\lambda^{2k} - \lambda^{2k} + k\lambda^{2k+2})$$

Hence, in this case, $H(G,\lambda) = H_1(G,\lambda)$.

One of the most frequent applications of the Hosoya polynomial is the calculation of the Wiener and hyper-Wiener indices. In fact

$$W(G) = \frac{d}{d\lambda} H(G,\lambda)\Big|_{\lambda=1}$$

and

$$WW(G) = \frac{1}{2}\frac{d^2}{d\lambda^2}[\lambda H(G,\lambda)]\Big|_{\lambda=1}$$

Since the polynomials are a continuity function, hence for the obtained polynomials one has:

$$W(G) = \lim_{\lambda\to 1}\frac{d}{d\lambda}[H(G,\lambda)]$$

and

$$WW(G) = \lim_{\lambda\to 1}\frac{1}{2}\frac{d^2}{d\lambda^2}[\lambda H(G,\lambda)]$$

Thus, one can calculate:

Result 4. The Wiener index of $HC_6[p,q]$ nanotori is given by:

$$\begin{cases} \frac{pq^2}{24}(-4+3p^2+3pq+q^2) \text{ if } q \le p \\ \frac{p^2q}{24}(-4+p^2+6q^2) \text{ if } q > p \end{cases}$$

Result 5. The hyper-Wiener index of $HC_6[p,q]$ nanotori is given by:

$$\begin{cases} \frac{1}{192}pq^2(-16+16p-20q+4p^3+6p^2q+4pq^2+12p^2+5q^3+4q^2+12pq) \text{ if } q \le p \\ \frac{1}{192}p^2q(3p^3+4p^2-12p-6+16q^3+24q^2+8q) \text{ if } q > p \end{cases}$$

CONCLUSION

A method has been developed which is usually very useful for calculating the Hosoya polynomials of C_6 nanotubes and nanotorus. As a consequence of calculating the Hosoya polynomials of zigzag polyhex nanotorus, the Wiener and hyper-Weiner of such nanotorous were computed.

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ИЗВОД

HOSOYA ПОЛИНОМ ЦИК-ЦАК ПОЛИХЕКС НАНОТОРУСА

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Hosoya полином молекулског графа G је дефинисан као $H(G,\lambda)=\sum_{\{u,v\}\subseteq V(G)}\lambda^{d(u,v)}$, где је $d(u,v)$ растојање између чворова u и v. Први извод од $H(G,\lambda)$ за $\lambda = 1$ једнак је Винеровом индексу графа G, који је дефинисан као $W(G)=\sum_{\{u,v\}\subseteq V(G)}d(u,v)$. Други извод

од $\frac{1}{2}\lambda H(G,\lambda)$ за $\lambda = 1$ једнак је хипер-Винеровом индексу, дефинисаном као $WW(G) = \frac{1}{2}W(G) + \frac{1}{2}\sum_{\{u,v\}\subseteq V(G)} d(u,v)^2$. Xu *et al.*[1] су израчунали Hosoya полином незатворених цик-цак наноцеви. Xu и Zhang[2] су израчунали Hosoya полином "armchair" незатворених наноцеви. У овом раду развијена је нова метода за одређивање Hosoya полинома за $G = HC_6[p,q]$, тј. за цик-цак полихекс наноторусе. Користећи $H(G,\lambda)$, израчунати су Винеров и хипер-Винеров индекс ових наноторуса.

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